

A CHanneled ION ENERGY LOSS STUDY
OF THE SURFACTANT-MEDIATED GROWTH OF GE ON SI(100)

By

MARK ANDREW BOSHART

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Abstract of Dissertation Presented to the Graduate School
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By

Mark Andrew Boshart

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Chairman: Lucy Elizabeth Seiberling

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Transmission ion channeling is used to investigate the surfactant-mediated growth of Ge on Si(100). The experimental scattered ion energy distributions for this system are compared with the simulated distributions for several models. The simulated distributions are obtained using a Monte Carlo simulation of channeling that incorporates channeled MeV light ion energy loss. A trial adsorbate site is then overlapped with the Monte Carlo output (ion position and energy within the channel at the exit surface).

To obtain a model for channeled ion energy loss, the energy distributions for 625 keV H^+ and 2.5 MeV He^+ ions incident on thin ($\sim 8000 \text{ \AA}$) Si single crystals are studied. Detailed angular scans are taken along low-index directions. Scattering is from an amorphous Au layer ($\sim 8 \text{ \AA}$) on the beam-exit surface. The experimental distributions are reproduced by a Monte Carlo simulation using the semi-classical

approximation model for energy loss to core electrons (scaled up 12%) and the 2-component free-electron gas model for energy loss to valence electrons (scaled down 6% and using the solid-state density).

A program for generating simulated energy distributions from the Monte Carlo output was developed by studying Sb on Si(100). The Sb site found agrees with previous experiments on this system, a modified bridge site with a bond length of 2.80 ± 0.10 Å and a distance above the bulk-extrapolated silicon surface of 1.63 ± 0.10 Å. The Sb vibrations appear anisotropic.

Finally, the surfactant-mediated growth of the system Ge/Sb/Si(100) is investigated. Coverages of 0.15 monolayer (ML) and 0.68 ML of Ge deposited at room temperature (RT) on Sb-terminated Si(100) are studied, both before and after annealing at 350°C. We find that RT deposition of Ge for both coverages is consistent with a model of loosely bonded Ge dimers adsorbed between undisturbed Sb dimer rows. After annealing, we observe bulk-like Ge underneath Sb dimers for 0.68 ML Ge. For 1 ML Ge deposited at 350°, the energy distributions clearly show that Ge is bulk-like, and the quantitative sites in the literature are consistent with the data.

CHAPTER 1 INTRODUCTION

Channeled Ion Energy Loss

The stopping of energetic ions in crystalline materials is known to strongly depend on the direction of incidence. In particular, ions moving along a major crystallographic axis lose their energy at a rate that can be as low as 50% or less of the so-called normal or random value. This reduced stopping is one of the dominant features of the channeling phenomenon [Morg73], and has fueled intense interest in the mechanisms of energy loss of channeled ions (i.e., for implantation applications). In contrast, the (well-studied in amorphous targets) random stopping occurs for directions far from any significant axial or planar channels, where the crystal lattice appears to the ion beam as a random-like arrangement of atoms.

The reduced stopping of channeled ions is easily understood in terms of the impact-parameter dependence of the energy loss that occurs in a single ion-atom collision. The channeled ions maintain large distances from the atom rows and, therefore, can only make small energy transfers to the atomic cores. Similarly, the contribution of valence (outer-shell) electrons to the stopping is diminished, as their density in the central region of the channel is reduced.

Investigations of energy-loss processes for ions interacting in single crystals have focused primarily on major axial and planar directions [Satt65; Satt67; Dell72; Eise75; Melv73; Cemb77; Carn78; Gehr85; Kita72; Dett74; Koma74; Dett75; Desa77; Esbe78; Bure80; Craw83; Kuhr83; Khod83; Gras85; Asco86; Gold86; Nami88;

Mort91], as the largest reduction in energy is achieved when aligned with these high symmetry directions [Gemm74]. The primary means of analysis of these early studies has been the high energy peak or leading edge value of the observed final ion energies (the energy distribution of the exiting ions) [Kuma81]. This gives a narrow view of the impact-parameter dependence of the energy loss as essentially only impact parameters close to the channel radius (the best channeled ions) are being explored. In addition, such comparisons are often ambiguous due to the inability to resolve various contributions to the energy loss [Belo78]. Further, an extraction of the leading edge value from experimental distributions is subject to uncertainties related to energy straggling and energy resolution factors [Stee81].

A much better method is to model individual trajectories in the crystal by the Monte Carlo technique, attempting to fit the full experimental distributions [Murt93; Dijk94], not just peak or leading edge values, allowing a study over a broader range of impact parameters. Furthermore, by tilting the crystal away from the axial (planar) direction, smaller impact parameters play an increasingly important role, and complex structures can be obtained in the energy distributions [Dygo94e]. The energy loss model thus proposed should be valid for impact parameters that span the channel radius rather than just near the channel center. An accurate determination of the energy loss processes for MeV light ions for impact parameters spanning the channel can then be employed by techniques that involve channeling.

Surfactant-Mediated Epitaxial Growth

To understand the importance of surfactant-mediated epitaxial growth, one must first understand the importance of and problems associated with strained layer

superlattices. Strained layer superlattices (such as Ge/Si heterostructures) are of extreme interest as they can be used as tools for modifying the band structures of materials. However, $>2\%$ strain (lattice mismatch) is required for significant band structure alteration [Pear90]. Further, interfaces must be largely defect free, thin ($\sim 100 \text{ \AA}$), and of uniform composition. Such superlattices can then be taken advantage of in lasers, bipolar transistors and field effect transistors to tune laser emission wavelengths and to improve transistor performance by the confinement of carriers [Pear90].

To grow strained layer superlattices with the required strain and uniformity is not an easy feat. Growing one material on another of course introduces strain as the two materials have different lattice constants. If the substrate free energy is larger than the interface plus grown layer free energy, then this elastic strain can, in general, be accommodated without defect formation to a certain point, as it takes energy to create dislocations. Thus, if the thickness of the grown layer is small enough, the energy required to relieve the strain by defect formation is larger than simply maintaining the elastic strain. This two-dimensional growth is referred to as Frank-van der Merwe growth. When a critical thickness is reached, defects will be produced to relieve the strain. One way of relieving the strain is for the material to grow in clusters, or islands, with its normal lattice constant, ruining the uniformity of the layer. This two-dimensional followed by three-dimensional growth is called Stranski-Krastanov growth.

Molecular beam epitaxy (MBE) has been extremely successful at achieving two-dimensional growth for up to 4% lattice mismatches, more than adequate for the applications noted above [Pear90]. However, defect production (islanding) limits

the thickness of the layers. Further, the alternating layer (the substrate layer from above) will not grow two-dimensionally at all, as its free energy will be too large. This layer will island immediately, referred to as Volmer-Weber growth.

The use of surfactants in creating high quality heteroepitaxial films has been of interest for several years [Cope89; Cope90; Eagl93]. For example, surfactants such as As and Sb are well known to aid in creating high quality Ge/Si heterostructures. The low energy, stable termination (due to the lone pair orbital which allows all bonds to be tied up) that these elements provide causes an overlayer, i.e. Ge or Si, to be rapidly incorporated into the bulk. Such an inhibition of the surface diffusion of Ge or Si is the basis of the high quality heteroepitaxial films; islanding is prevented and layer-by-layer growth is achieved for both Ge grown on Si and vice versa. The use of surfactants also increases the critical thickness for the onset of defect formation, and improves the crystallinity for thick layers (~ 100 nm). Some incorporation of the surfactant into the superlattice is observed (as little as 1% incorporation of Sb in a $100 \text{ \AA}$ grown layer can affect electronic properties), but a good surfactant choice will segregate to the surface with high efficiency (group V elements) [Cope89].

The fact that surfactant-mediated growth provides abrupt interface heterostructures is well-documented [Saka92; Oste92; Cao92; Oste93]. However, the microscopic details of the site exchange processes between Ge/Si and the surfactant are not well-understood. Further, the exact Ge/Sb locations after site exchange have not been extensively quantified [Gran94c].

Motivation

Advantages of Using Transmission Ion Channeling

Transmission ion channeling has proven to be a powerful tool for the study of interface reactions and adsorbate registry with the substrate [Cheu79; Cheu80b; Jin85; Lyma91b; Seib87]. In particular, transmission ion channeling can be used to determine the adsorption site of atoms on a surface [Cheu81; Sten85; Jens90; Gran92; Gran94b; Gran94c]. Adatoms near substitutional sites can be differentiated from their interstitial counterparts with little or no data analysis. More quantitative site determination requires comparison of experimental data with calculations. Typically, transmission ion channeling data have been compared to results of an analytic calculation that employs the continuum approximation [Jens90], treating strings of atoms as lines of charge. The ion flux distribution as the beam exits the crystal near high-index directions of the substrate is calculated and overlapped with trial adatom sites, resulting in a calculated scattering yield versus tilt from the high-index direction. Such a method of analysis can typically give the adsorbate location with respect to the underlying substrate atoms with a resolution of 0.1 Å [Seib93].

Advantages of Using a Monte Carlo Simulation of Channeling

A common method to simulate channeling, as mentioned, is to use the continuum approximation [Lind65]. Atom rows are approximated by lines of charge, and the potential in the channel is readily calculated. One such simulation of channeling by Bech Nielsen [Niel88b] uses a thermally averaged multi-string Doyle-Turner potential. It assumes statistical equilibrium; a particle is equally likely to be anywhere in its energetically accessible area. Dechanneling is included (see Chapter

2) [Bond72]. We employed this simulation using the 2D RMS thermal vibrational amplitude ($\rho = \sqrt{2}u$, where u is the 1D vibrational amplitude) of silicon, 0.11 Å at room temperature, and a beam divergence of 0.03°.

A more accurate method of analysis involves the modeling of individual ion trajectories within the crystal by the Monte Carlo technique [Barr71]. In a Monte Carlo simulation of channeling, a large number of individual ion trajectories are followed in the crystal, taking into account as many interactions as possible, as accurately as possible. We employed the CXX simulation code [Dygo88; Dygo89; Dygo94c; Dygo94d] to calculate channeled ion trajectories. The code made use of the He-Si interaction potential based on the Hartree-Fock electronic density modified for solid-state effects [Dygo92; Smul92]. The silicon 1D vibrational amplitude of 0.078 Å was assumed for three dimensions and an incident beam angular divergence of 0.03° was included as well as multiple scattering by electrons.

In Fig. 1-1, a comparison of the two methods is made. The ion fluxes of the two models were overlapped with a bulk silicon position. At first glance, it appears that neither of the calculated yields reproduces the data very well. However, the data represent the entire silicon signal ($\sim 1 \mu\text{m}$), not just the signal obtained as the ions leave the crystal, as is assumed in the calculations. Thus, one must conclude that the Monte Carlo simulation, residing as it does above the data, is more representative since the ion flux is expected to smooth out from dechanneling after large penetration depths. This test case represents the worst case scenario for the continuum approximation; ions traveling close to atom rows, able to scatter from bulk sites will not feel lines of charge, but the graininess of the potential [Gemm74]. A further weakness of the analytic calculation is that statistical equilibrium can be

satisfied only if there are no planar effects; azimuthal averaging must be performed in the experiment [Smul90]. Therefore, although time consuming due to the large number of individual trajectories that must be followed, a Monte Carlo simulation has clear benefits.

Advantages of Using Energy Distributions

The Monte Carlo approach has an extra benefit. Ions penetrating single crystals, especially near high-index directions, do not sample all impact-parameters equally (as for random incidence). As one follows an ion through in the Monte Carlo simulation, one calculates all the sampled impact parameters. Thus, if one can successfully model the impact-parameter dependence of the energy loss of MeV light ions, a Monte Carlo simulation can not only calculate ion positions within the channel as they exit the crystal, but also their exit energy. This additional information can also be used to test trial adatom sites through the generation of simulated energy distributions for specific adsorbate sites; adatoms near substitutional locations and those at interstitial sites will produce very different energy distributions. For example, near-substitutional adatoms can only interact with ions spending time near atom rows, which selects ions that lose more energy than those staying near the channel center, due to the smaller sampled impact parameters.

The use of energy distributions for site determination is novel, and a brief discussion of how the procedure works should be undertaken. Figure 1-2 gives a good idea of how the procedure works from a qualitative viewpoint. Shown are four $\langle 100 \rangle$ channels (the large black dots indicate the Si atom rows that define the channels and the different sizes give an indication of how close the top Si atom in that row is to the surface). The small dots within the channels are ion positions

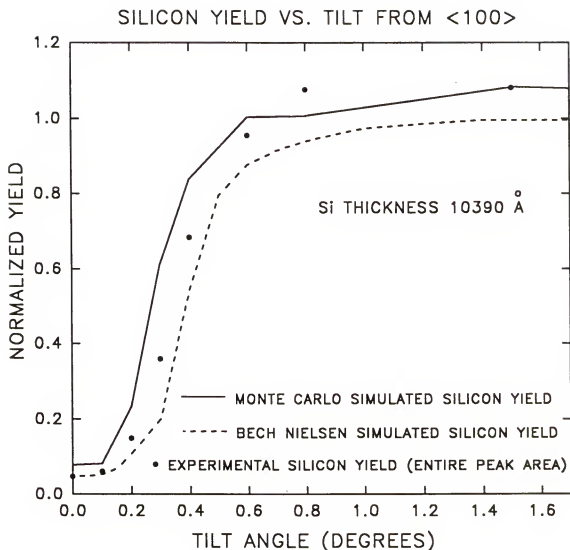
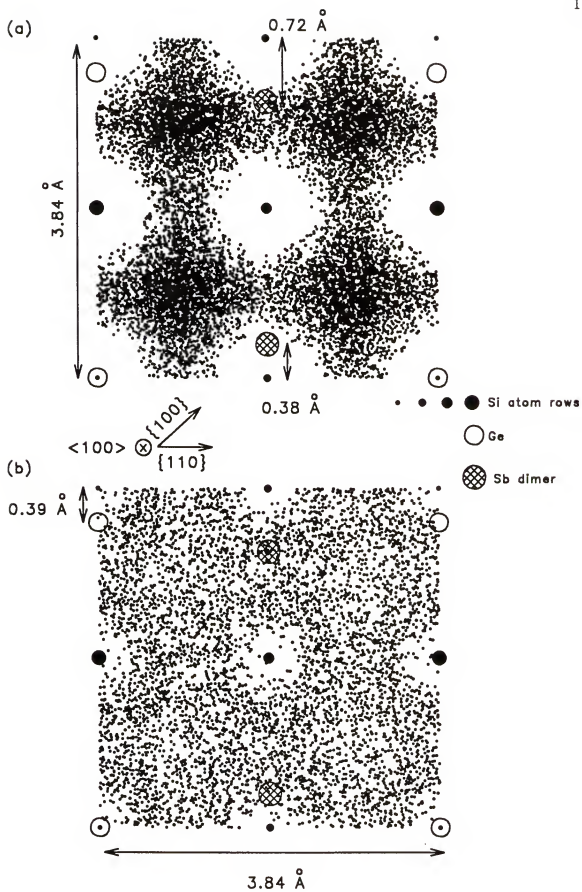


Figure 1-1. Comparison of a Monte Carlo calculated (solid lines) bulk silicon yield (obtained as the beam exits the crystal) versus tilt from the $\langle 100 \rangle$ axis with the analytic calculation (dashed lines) of Bech Nielsen which employs the continuum approximation. Both simulations assume a 2D silicon vibrational amplitude of 0.11 Å and an angular beam divergence of 0.03° . Experimental data (dots) are taken from the entire silicon signal ($\sim 1 \mu\text{m}$).

after penetrating the Si crystal aligned with the $\langle 100 \rangle$ axis. Figure 1-2(a) shows ions that have retained more energy (by $\geq 30\%$) than that expected if the crystal had been aligned at “random” incidence with the same crystal thickness ($\sim 1800 \text{ \AA}$). These ions are clearly very well channeled. Figure 1-2(b) shows all other ions, and some channeling is still evident, but these ions are able to penetrate close to the atom rows (which is responsible for their higher rate of energy loss). Thus, an adatom site encounters a very different range of energy and number of ions depending on where it is located within the channel (the greatest sensitivity is achieved near the middle of the channel, where fluxes are changing rapidly with channel position). The experimental energy distribution as well as overall yield (with respect to random incidence) typically give a resolution of $\sim 0.1 \text{ \AA}$ for the adatom site [Bosh95c].

For example, Fig. 1-2 also shows the positions of Ge and Sb found in a study by Grant *et al.* [Gran94c]. The Ge atoms are represented by the hollow circles occupying near-substitutional sites (half are substitutional). The overlying Sb dimer is represented by the cross-hatched circles. It is immediately noticed that low energy loss, well-channeled ions are not sensitive to near-substitutional positions (Fig. 1-2(a)). However, a substantial increase in overlapping ions is evident for these sites in Fig. 1-2(b), with the higher energy loss ions penetrating close to the atom rows. This results in a large yield difference ($\sim 25\%$) as well as a difference in energy of overlapping ions (resulting in a peak shift in the energy distribution that depends on the sample thickness) between completely substitutional sites and those displaced by as little as $0.1 \text{ \AA}$ from substitutional. This sensitivity to near-bulk positions using a Monte Carlo simulation with channeled ion energy loss is enhanced over previous transmission channeling studies that employ the continuum model.

Figure 1-2. View of the Si(100) surface from above. Large black dots are Si atom rows and small dots are ion positions when exiting the Si crystal. In (a), well-channeled low energy loss ions are shown (see text), while (b) shows ions with higher energy loss. Open and cross-hatched circles are Ge and Sb positions according to Ref. [Gran94b]. Proposed sites are evaluated by overlapping the site with the ion flux and comparing with experimental data. Higher energy loss ions penetrating close to atom rows are sensitive to near-bulk sites.



The continuum model excludes ions that penetrate close to atom rows and displacements of a minimum of $0.1 \text{ \AA}$ (the size of bulk vibrations) from bulk sites are necessary for sensitivity to those displacements [Niel88a].

Since we have established that a Monte Carlo simulation to generate ion positions and energies is advantageous (for adsorbate yield and energy distribution calculations), we consider the use of the energy distribution fit in addition to the scattering yield fit for a trial site. After all, the two are intimately related; aligned with a high symmetry direction, incident ions are steered into the middle of the channel by the atom rows where they experience reduced stopping due to the large impact parameters (reduced electron density). Thus, an adsorbate site with a peak in scattering yield due to a position near the middle of a channel will also have relatively high energy ions scattering from it; the information appears redundant. However, there are some distinct advantages in using the energy distributions in concert with the scattering yields to obtain adsorbate site information. First of all, the scattering yield is sensitive to beam-induced desorption of the adsorbate [Gran92] as well as current integration inaccuracies, while the energy distributions are not. Secondly, the energy distributions can exhibit complex shapes [Dygo94e; Dygo94f; Bosh95b], and if the beam-sample system is well-calibrated, these shapes can be fully taken advantage of for improved resolution in site location over just the scattering yield information. Finally, if an adatom site is already suspected from another study, the energy distributions appear sensitive to anisotropic vibrational amplitudes [Bosh95c].

As an overview, we will tie together what has been addressed. The use of transmission ion channeling is a good technique for identifying adsorbate registry

with a substrate. The data analysis using this technique should be undertaken using a Monte Carlo simulation of channeling to accurately pinpoint adsorbates near substitutional sites. This dissertation will address the impact-parameter dependence of channeled ion energy loss, and this can be incorporated into the Monte Carlo simulation to aid in adsorbate location by energy distribution simulation of specific adsorbate sites. Finally, using this novel technique of energy distribution simulation, this dissertation will investigate the surfactant-mediated growth of Ge on Si(100).

CHAPTER 2

TRANSMISSION ION CHANNELING

In this chapter, we will introduce the technique of transmission ion channeling as it is used in our laboratory. This will include a description of the laboratory equipment and an introduction of the fundamental principles of Rutherford Backscattering and channeling. Then we will discuss the use of transmission channeling for adsorbate site location as it is usually applied (and has been by us).

Equipment

The equipment in our laboratory has been extensively discussed elsewhere [Lyma91a; Gran94a]. Here, we present the key features of our lab. The accelerator is a 3.5 MV Van de Graaff accelerator. It can produce both H^+ and He^+ beams with high current ($1\mu A$ beams are readily achievable, but not desired due to pulse pile-up and radiation damage). The analyzing magnet selects beams using an NMR probe, and a switching magnet selects from among five beamlines (only two are currently being used).

Our lab is equipped with two ultra-high vacuum (UHV) chambers and an introduction chamber kept at high vacuum (see Ref. [Seib93]). UHV conditions are attained by baking the chambers at about $120^\circ C$. After the Si thin windows have been prepared and cleaned (see Appendix B), the windows are mounted onto Ta modules with screw down clips to hold the sample in place. The modules are then placed into the introduction chamber. The chamber is pumped down using

a sorption pump for roughing and an ion pump that is continually run to maintain the vacuum (this is similar on the other chambers).

Transfer arms are used to transfer the modules between chambers under vacuum. When an experiment is to be performed, a sample is transferred from the introduction chamber to the preparation chamber, where it resides on a manipulator which can be moved throughout the chamber interior (two angular and three translational degrees of freedom). This chamber is equipped with analytical and sample preparation tools: Low Energy Electron Diffraction (LEED), Auger Electron Spectroscopy (AES), a sputter gun, and Ge and Sb effusion cells. Further, the manipulator has a Ta (resistive) heating strip behind the sample (sapphire shielded) and there is also a heat lamp (Tungsten-halogen bulb in an elliptical reflector) inside the chamber.

The sample is now placed in front of the heat lamp at the point of focus (determined previously) and the lamp is turned on to low (6 A) current. This procedure allows the sample to degas without desorbing the protective oxide and attaining the clean surface prematurely. This takes a couple of hours. The current is now raised to around 8 A in an attempt to desorb the oxide. The pressure is not allowed to exceed 1.5×10^{-9} Torr, and heating is allowed to continue for about 10 minutes. The LEED pattern is now checked, and the process is repeated until the expected sharp 2×1 pattern for Si(100) is obtained of sufficient size (the sample size is ~ 1 cm $\times$ 1 cm) [Gran94a].

The clean sample is now placed in front of an effusion cell to deposit Ge or Sb (or both). The water-cooled effusion cells operate like ovens (Ge is heated to 1150°C, and Sb to 600°C), with the material coming out in a jet through a small opening

[Lyma91a]. The sample can be heated during deposition using the Ta strip if this is desired. Deposition rates must already have been properly calibrated. LEED is now checked again, and if everything appears okay (expected LEED patterns of sufficient size), the sample is transferred to the scattering chamber, again using transfer arms.

The scattering chamber is 6 inches in radius. It contains three bakeable, passivated, ion-implanted silicon detectors (see Chapter 4), and a goniometer with two angular degrees of freedom and translations in three dimensions. It is connected to the accelerator by differential pumping along the beamline. Pressures in the scattering chamber can be maintained at 2×10^{-10} Torr with the beam on sample. The beam is centered through the goniometer with quadrupole (focusing) and steering magnets before the sample is transferred. Beam size is 1 mm x 1 mm, with an angular divergence of 0.03° , attained by standard aperture and slit (to cut out scattering from the aperture) collimation.

The sample is placed on the goniometer with the adsorbate layer facing the beam, and Rutherford Backscattering is performed to locate spots (up to five spots are available) on the sample with the desired adsorbate coverages. The sample is then turned around for transmission ion channeling experiments. Beam dose on the sample is monitored by a Faraday cup at the end of the beam-line (isolated from the rest of the chamber).

MeV Ion Scattering

Rutherford Backscattering Spectrometry (RBS) has been used extensively as an analytical tool [Chu78]. The well-known cross section and energy loss processes make this technique indispensable for areal density calculations and depth profiling.

In addition, if single crystal substrates are involved, channeling can be employed in conjunction with RBS to study interface defects, implantation, thermal vibrations, etc. In this section we will look at the features of RBS that will be useful to us throughout this dissertation. We will also introduce the basics of channeling, the primary technique employed in this research.

Rutherford Backscattering Spectrometry

Kinematic Factor. The basic problem that we are dealing with is that of a particle of mass M_1 colliding elastically with a particle of mass M_2 , as we are accelerating particles and directing them at a target (the problem is classical due to the small de Broglie wavelength, 8×10^{-15} m, and elastic as nuclear reactions are avoided). Thus, we can employ the conservation of energy and momentum to obtain the ratio of the incident particle's final energy, E_1 , relative to its initial energy, E_0 , given the masses of the particles and the angle at which the incident particle scatters θ [Chu78]. This quantity we will refer to as the kinematic factor, K ,

$$K \equiv \frac{E_1}{E_0} = \left[\frac{(M_2^2 - M_1^2 \sin^2 \theta)^{\frac{1}{2}} + M_1 \cos \theta}{M_2 + M_1} \right]^2. \quad (2-1)$$

The kinematic factor is essential because the scattering angle is defined by the detector position, the masses of the species are known, and the initial energy of the incident particles is set by the accelerator. When scattering from the target occurs near the surface of the target (before the incident particles lose energy by penetrating into the target), the energy of the particle after scattering is well-known.

Rutherford Cross Section. Another important principle is that of probability of an incident particle scattering off a target atom at a given angle. At the incident

particle energies that we use (~ 2 MeV), the differential scattering cross section derived by Rutherford applies [Chu78],

$$\left(\frac{d\sigma}{d\Omega}\right)_c = \left[\frac{Z_1 Z_2 e^2}{4E_c \sin^2(\theta_c/2)}\right]^2, \quad (2-2)$$

where $d\Omega$ is the differential solid angle, Z_1 and Z_2 are the atomic numbers of the incident and target particles, respectively, e is the electronic charge ($e^2 = 14.4 \text{ eV} \cdot \text{\AA}$) θ is the scattering angle, and E is the energy of the projectile immediately before scattering. The subscript c denotes center of mass coordinates (if $M_2 \gg M_1$, usually the case, the c can be ignored as center of mass and lab coordinates approach one another).

In order to take into account the finite size of the detector (though with θ still well-defined), we introduce the average differential scattering cross section, σ [Chu78],

$$\sigma \equiv \left(\frac{1}{\Omega}\right) \int_{\Omega} \left(\frac{d\sigma}{d\Omega}\right) d\Omega. \quad (2-3)$$

Of course, for detectors with a very small solid angle ($\Omega \sim \text{msr}$), $\sigma \rightarrow \frac{d\sigma}{d\Omega}$.

Energy Loss and Straggling. The final basic concept important for Rutherford Backscattering Spectrometry (RBS) is that of energy loss per unit path length and straggling of the incident particles as they traverse the target. The energy loss per unit path length, $-\frac{dE}{dx}$ (also called stopping power), due to momentum transfer from the passing particle to electrons in the target (close collisions) was calculated similarly by Bohr [Feld86],

$$-\frac{dE}{dx} = \frac{2\pi Z_1^2 e^4 n}{m_e v^2} \ln \frac{2m_e v^2}{I}, \quad (2-4)$$

where n is the number of electrons per unit volume, I is the excitation energy of an average electron, and v is the velocity of the incident ion. There is a term

comparable in size due to distant resonant energy transfer, resulting in a stopping power about twice that shown in Eq. 2-4 [Feld86].

This picture of energy loss is a decent approximation for helium incident ions at typical Rutherford Backscattering energies ($\sim$ MeV's) because relativistic effects can be ignored, and nearly all target electrons are involved in the stopping process (tightly bound inner shell electrons for high atomic number targets must be treated differently) [Feld86]. In practice, though, it is necessary to use tabulated values based on experimental results. MeV helium ions into silicon have been extensively studied (amorphous targets are typically used so channeling effects can be ignored), and the stopping power is known in our energy range to within 5% [Zieg77b].

The experimental results are fit to a functional form with several parameters. It is then straightforward to find the stopping power at any energy by plugging into the numerical fit. An iterative calculation will then yield the ion energy at an arbitrary depth into the target.

As a particle traverses the target, however, the energy that it loses due to individual encounters will be influenced by statistical fluctuations [Feld86]. Thus, two incident helium ions traversing identical target thickness will probably not have identical energies. This effect is called energy straggling, with the dominant contribution being due to fluctuations in stopping due to electronic collisions. The distribution in energies is approximately gaussian, with a standard deviation Ω_B ,

$$\Omega_B^2 = 4\pi Z_1^2 e^4 n t, \quad (2-5)$$

where t is the target thickness penetrated. It is important to note that the degree of straggling depends on the penetration depth. Again, in principle it is necessary to yield to experimental results to obtain accurate straggling values [Yang91].

Obtaining an Energy Spectrum. With the basic backscattering principles that have been outlined, we are now in a position to look at a typical backscattering energy spectrum and how it is obtained. In order to detect a scattered ion, a reverse bias is placed on a solid state Si surface barrier detector [Tesm95]. Thus, a current will only register when electron-hole pairs are generated randomly in the depletion region, due to an incoming ion depositing its energy (by electronic energy loss mechanisms) in that region. The collected charge is linear with loss of energy of the penetrating ion, so the total collected charge is proportional to the energy of the detected ion. This signal is then pre-amplified and amplified into a pulse whose height is proportional to the energy of the detected ion. Using standard pulse height analysis, the energy spectrum is thus obtained with a personal computer based multi-channel analyzer (Canberra), with channel number representing the height of the incoming pulse. Typical energy resolution is 15–20 keV.

The length of time for data collection is determined by the incident beam dose on the sample. If the scattering chamber is isolated, current integration is straightforward. The current integrator then sends a signal to a pulser, which is connected to the pre-amplifier. Thus, current integration can be achieved by monitoring the peak height of the pulser signal. A typical backscattering energy spectrum is taken for $\sim 10 \mu\text{C}$ of incident beam dose, taking about 15 minutes depending on the beam conditions. A correction to the current integration must be made to take into account the equilibrium charge state of the helium ions (1.94) upon exiting the silicon crystal [Lyma91a]. After penetrating the sample, the He^+ ions rapidly become almost completely stripped (see Chapter 3), and current integration takes place at the end of the beam-line, after the ions have traversed the sample.

Figure 2-1 shows a backscattering spectrum for 2.5 MeV He^+ ions impinging on a thin ($\sim 10 \text{ \AA}$) Au gold layer deposited on a silicon substrate ($\sim 8000 \text{ \AA}$). The spectrum was collected for $4 \mu\text{C}$ of incident beam dose, monitored by the pulser peak located to the far right in the spectrum, away from the incoming data. Just to the left of this pulser peak is the peak from the thin Au layer on the surface. Further left is the signal from the silicon substrate. It is wide because the substrate is much thicker than the Au layer.

Much information can be garnered from this simple backscattering example given the basic principles outlined above. Outlining the general features of the spectrum, we first note that the location of the Au and Si (high energy side) signals is determined solely by their kinematic factors as incident beam energy and scattering angle are fixed. Due to finite detector resolution, the half-height of the silicon signal is chosen for the “peak” location. Second, the height of the signal is determined by the probability of a scattering event, dictated by the Rutherford cross section and target areal density as dose and solid angle are fixed (detector resolution also factors in). Further, the Si signal increases somewhat at lower energies due to the incident beam losing energy as it penetrates the substrate, increasing its probability of scattering. Finally, the low energy side of the Si signal displays somewhat poorer resolution than the high energy side due to energy straggling.

Calibrating the Energy Axis. It is necessary to convert the channel number in the raw data to an energy as we will be dealing with helium ion energy distributions later. This is a straightforward procedure as the kinematic factors of the various elements in the spectra are known and the scattering angle and incident beam

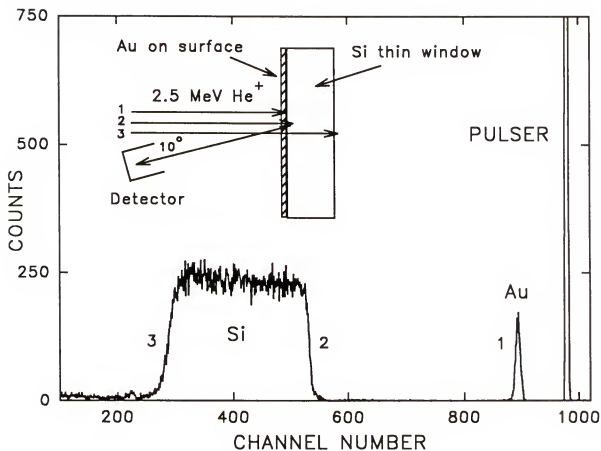


Figure 2-1. Raw backscattering data for Au on a Si thin window. The Au and Si peak positions are determined by their kinematic factors. Peak heights are determined by the Rutherford scattering cross section, and the increase in Si height at lower energies is due to the $\frac{1}{E^2}$ dependence of the cross section. As the beam penetrates further into the sample, it loses energy and has a greater scattering probability. The scattering geometry is also shown, and important scattering points are displayed. Points 1 and 2 allow conversion from channel number to energy, and 3 allows a Si thickness determination.

energy are fixed,

$$E_1 = K E_0. \quad (2-6)$$

However, one must be careful to obtain signals near the surface as ions penetrating into the target will suffer additional energy losses and Eq. 2-6 will not yield the correct energy of the ions.

Since the channel number is linearly related to the energy of the scattered ion, we need two points to obtain the energy calibration. Referring once again to Fig. 2-1, this is readily obtained from the Au peak and half-height of the high energy edge of the Si signal (points labeled 1 and 2). Both of these signals are obtained close enough to the surface so that Eq. 2-6 applies. In practice, the energy calibration is performed by a FORTRAN program, ECALIB.FOR [Bosh93a], which accepts atomic symbols, scattering angle, beam energy before scattering, and channel numbers as input and calculates the energy calibration in the form of

$$\text{energy (keV)} = \text{slope} \left(\frac{\text{keV}}{\text{channel}} \right) \times \text{channel number} + \text{intercept (keV)}. \quad (2-7)$$

If more than two elemental species are available, the program will try all combinations of elemental pairs, and the most consistent fit is used. Table 2-1 demonstrates the process.

Table 2-1. Demonstration of ECALIB.FOR. The incident helium ion energy is 2500 keV, and the scattering angle is 170°. The energy calibration is 2.48 keV/ch + 93.1 keV.

Element	K	E_1 (keV)	Peak (Edge) Channel Number
Si	.5658	1415	533.5
Au	.9225	2306	893.5

Silicon Thickness. We will also find it important to know the thickness of our silicon substrate. This is readily accomplished once we have obtained the energy calibration. The channel number corresponding to the half-height of the low energy side of the silicon signal (illustrated by point 3 in Fig. 2-1) is read off from the spectrum and converted to an energy utilizing the energy calibration. This point corresponds to scattering from the back side of the silicon signal (inset of Fig. 2-1) and since the helium beam penetrates deep into the target, the energy lost by the beam as it traverses the target must be taken into account. If this energy loss is known, then by guessing the path length (essentially trying a silicon thickness) and comparing to the energy obtained from ions that scatter from the silicon back surface, the thickness can be obtained.

This task is accomplished using the program HESTOP.FOR [Bosh93b], which makes use of the experimental energy loss measurements for helium ions incident on amorphous silicon and fit to a functional form [Zieg77b]. The energy loss rate depends on the energy of the ion, so an iterative calculation is necessary. That is, the stopping power is calculated (around $21 \frac{\text{eV}}{\text{\AA}}$ for 2.5 MeV He^+), and a penetration depth to update the energy loss rate is chosen (the step-size usually chosen is 1 $\text{\AA}$). The ion energy can now be updated by subtracting the resulting energy lost by the ion in moving one step through the target. The energy loss rate must be recalculated now since the ion energy has been reduced. The process is outlined in Table 2-2.

When the iteration reaches the inputted silicon thickness, the ion energy must be reduced by the kinematic factor for helium on silicon (or any element that happens to be on the beam-exit surface) due to the actual close encounter which scatters

Table 2-2. Demonstration of HESTOP.FOR. The incident helium ion energy is 2500 keV, and the path length through the silicon target is 5000 Å.

Penetration Depth (Å)	Energy	$-\frac{dE}{dx} \left(\frac{eV}{\text{Å}} \right)$
0	2500	21.4
1000	2479	21.6
2000	2457	21.6
3000	2435	21.7
4000	2413	21.8
5000	2392	21.9

the ion into the detector. Then the ions must traverse the crystal once again back to the detector, with the iterative energy loss calculation continuing, but the path length must be increased (by $\frac{1}{\cos \theta}$, where θ is the scattering angle) due to the geometry of the event (inset of Fig. 2-1). Further geometrical effects are taken into account if the beam isn't incident normal to the silicon surface (Fig 2-2). Silicon thicknesses are tried until the calculated ion energy matches that obtained from the energy spectrum.

Species Coverage. Finally, RBS is extremely good for obtaining target areal densities [Chu78]; the number of detected particles is proportional to the number of incident particles times the number of target atoms per unit area (proportionality is the probability of recording a scattering event). Or,

$$A = \sigma \Omega Q N t, \quad (2-8)$$

where A is the number of detected particles, Q is the total incident dose, σ is the probability of a scattering event (the average Rutherford cross section), Ω is the solid angle of the detector, N is the volume density of target atoms, and t is the thickness of the target layer (Nt is the areal target density, then). The number

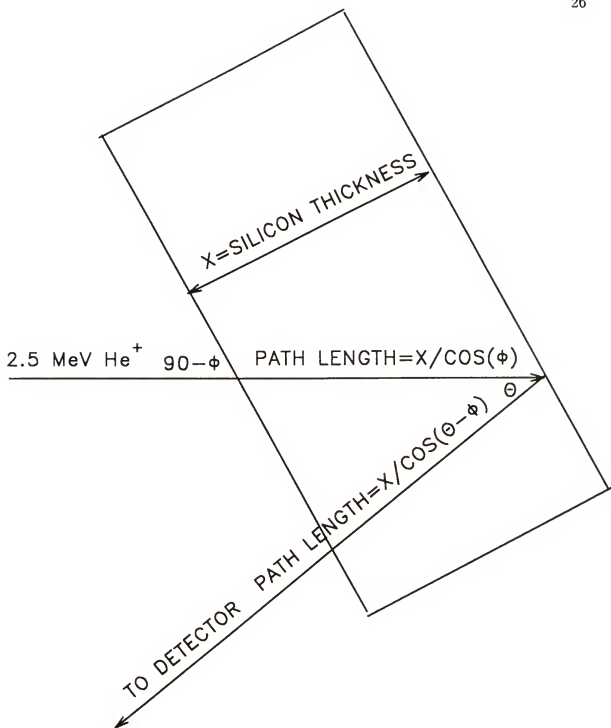


Figure 2-2. Geometry for beam-sample-detector system necessary for calculation of silicon substrate thickness. The angle between the beam and sample normal is $90 - \phi$, and the scattering angle (angle between beam and detector) is θ . By knowing these angles and trying various sample thicknesses, X , and, thus, various beam path lengths, the substrate thickness can be calculated from energy loss considerations.

of detected particles is obtained by summing the peak of interest in the energy spectrum, so the areal target density is readily obtained, and is accurate to better than 10%. This information can be used to obtain substance thicknesses if the density of the material is known by some other method (or assumed).

Channeling and the Continuum Model

Channeling occurs when a beam of energetic ions is incident on a crystalline material near a low index direction (a direction of high symmetry). The ions undergo a series of small angle collisions with the atom rows (or planes) due to the screened Coulomb repulsion [Tesm95]. The result is a steering toward the middle of the space between the atom rows (referred to as a channel). Figure 2-3 shows a beam incident along a high symmetry axis. The small open circles represent atoms making up an atomic row (the scale is greatly exaggerated). The incident beam is steered back and forth between the atom rows, with an amplitude determined by where the ion entered the channel. The closer the ion enters to the atom row, the greater the deflections (larger repulsion). However, the incident ion beam uniformly covers the entire channel, so most ions will be away from atom rows and will undergo small amplitude collisions.

The net result of this is called flux peaking. All of the channeled ions (ions not incident right along an atom row, roughly 96% of the incident ion beam, and thus dechanneled by a large angle collision) spend time near the channel center. However, few ions spend time near the atom rows, so a nonuniform ion flux which is peaked at the channel center results. It is of great use to be able to calculate this flux peaking as it will be the basis for most of what follows.

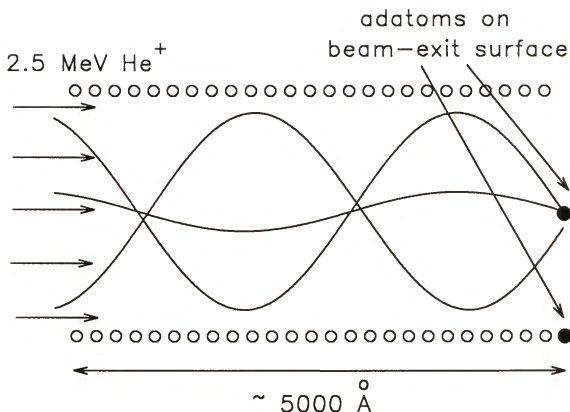


Figure 2-3. Steering of the incident ion beam by the atom rows. Ions incident near the atom rows experience large amplitude steering, while those incident near the channel center (most ions) are gently steered. Flux peaking in the channel center is a result of the fact that all ions spend time near the channel center, while few spend time near the atom rows. Interstitial adsorbates will thus have enhanced scattering yields, and substitutional adsorbates will experience reduced scattering (relative to “random” incidence).

In order to understand the channeling phenomenon, let us consider the atomic rows to be lines of charge with a uniform charge density (continuum model) [Lind65; Niel88a] (planes can be treated in a similar fashion),

$$U(\vec{r}) = \frac{1}{d} \int_{-\infty}^{\infty} V^{\text{at}}[(r^2 + z^2)^{\frac{1}{2}}] dz, \quad (2-9)$$

where $U(\vec{r})$ is the potential describing the collision with the string, d is the distance between atoms along the string, and V^{at} is the screened atomic potential [Niel88a]. Since the potential depends only on the distance to the string, $|\vec{r}|$, the energy transverse to the motion is conserved,

$$E_{\perp} = E\theta^2 + U(\vec{r}). \quad (2-10)$$

Here, θ is the angle that the incident beam makes with the axial direction, so $E\theta^2$ is the kinetic energy perpendicular to the string, and $E_{\perp}$ is the total energy perpendicular to the string.

The above is the basis for a channeling simulation written by B. Bech Nielsen [Niel88a; Niel88b] (and used by our group for data analysis in the past) [Gran92; Gran94b; Gran94c]. The potential chosen is a multistring, thermally averaged Doyle-Turner potential. Twenty-five atom rows are included in the calculation of the potential in the three major axes in Si (the $\langle 100 \rangle$, the $\langle 110 \rangle$, and the $\langle 111 \rangle$). The grid density for the calculation is 100×100 , with the grid size depending on the channel. The program then divides up the channel into several (~ 40) equipotentials, and assuming a uniform beam, the program calculates the number of particles falling into each equipotential.

Now, based on Eq. 2-10, a particle cannot leave its accessible area (it cannot move to a higher equipotential), however, a particle is assumed to be equally

likely to reside anywhere in its accessible area (statistical equilibrium). Dechanneling is included in the calculation (allowing the particles to change their accessible area) through a diffusion-like equation for the ion energy distribution transverse to the atomic rows. Dechanneling from interactions with electrons and host nuclei is considered. In this way, the number of particles versus accessible area (equipotential) is built up, the ion flux distribution in the channel. The crystal thickness enters by determining the amount of dechanneling to consider. The flux at the beam-exit surface is then obtained, $(g(E_{\perp}, z))$, where z is the crystal thickness) and this is what we will need for the adsorbate location in the next section.

It can be seen that for ions penetrating close to the atom rows, the continuum model breaks down. This is because such ions will see the graininess of the potential, not lines of uniform charge. It has been estimated [Niel88a] that the continuum model can be applied even for these cases if host atom vibrations are large enough in the transverse plane (Si meets the criterion). However, underestimations in the yield for substitutional (host atom) sites when aligned with axial directions are observed (see Chapter 1). Further, the energy lost by the channeled beam is ignored.

Yield Versus Tilt for Adsorbate Location

We must now calculate the yield that an adsorbate will generate given the flux distribution $g(E_{\perp}, z)$ and the adsorbate position within the channel. If the adsorbate location is taken to be gaussian around an equilibrium position (standard deviation $\frac{1}{\sqrt{2}} \rho$, where ρ is the 2D vibrational amplitude, see Chapter 5), then the yield can be calculated by the overlap of this position with the ion flux,

$$\chi(E, \theta, z) = A_0 \int_0^{\infty} g(E_{\perp}, z) \left(\int F_a(E_{\perp}, \vec{r}) P_i(\vec{r}) d\vec{r} \right) dE_{\perp}. \quad (2-11)$$

Here, χ is the calculated yield, $P_i(\vec{r})$ is the location of the vibrating adsorbate, $F_a(E_\perp, \vec{r}) = 0$ if $U(\vec{r}) > E_\perp$ (inaccessible region) and $F_a(E_\perp, \vec{r}) = \frac{1}{A(E_\perp)}$ if $U(\vec{r}) < E_\perp$ (statistical equilibrium, $A(E_\perp)$ is the area of an equipotential), and A_0 is the total area of the channel [Niel88a].

The result of all of this is shown in Figs. 2-3 and 2-4. The black dots at the beam-exit surface in Fig. 2-3 represent interstitial and substitutional adsorbate sites. Adsorbates located near channel centers will overlap much larger ion fluxes than those located near atom rows for the simple reason that all of the particles are able to access the channel center (Eq. 2-10), the basis for flux peaking (see above). Figure 2-4 shows calculated yields versus tilt (angular scans) from the axis for interstitial, substitutional, and amorphous sites. As mentioned, the interstitial sites enjoy greatly enhanced scattering yields, while their substitutional counterparts encounter very few incident ions. The amorphous (incommensurate) site averages out the two effects and results in a flat scan. As tilt increases, more and more regions are accessible to all ions (Eq. 2-10), and the flux peaking effect diminishes until all yields are at the “random” (non-aligned) level.

Thus, if an adsorbate displays anything other than a flat scan, it is commensurate with the substrate in some way, and we can try to isolate its registry with the substrate. By direct comparison of experimental and simulated angular scans, the adsorbate location relative to the host crystal can be determined to within 0.1 Å [Seib93].

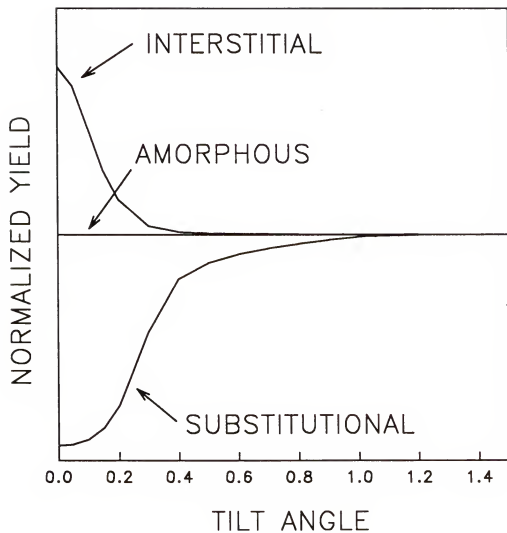


Figure 2-4. Yield versus tilt (angular scan) for various adsorbate sites (a result of flux peaking). Interstitial adsorbates overlap high flux areas and give a peak in the yield, while substitutional adsorbates result in a yield dip. Flux peaking levels off with tilt from the high symmetry direction, and the yield approaches that for “random” incidence. Amorphous or incommensurate adsorbates have flat scans as they average out the flux peaking.

CHAPTER 3 ENERGY LOSS OF CHANNELED MeV LIGHT IONS IN SILICON

Van de Graaff Calibration

It is of crucial importance to know as well as possible the energy of the incident beam, as all data analysis in this dissertation assumes that this is known. The incident energy is determined by measurement of the analyzing magnet field with an NMR gaussmeter. Using the $^{27}\text{Al}(p, \gamma)$ resonance reaction at 991.9 keV [Tesm95] (per H) for H^+ and H_2^+ , and noting the frequency of the NMR probe at the onset of resonance, one can calibrate the analyzing magnet as there is a linear relationship between magnetic field and NMR probe frequency. The onset of resonance is determined by counting the γ yield in a NaI detector at various NMR frequencies for a constant ($40\mu\text{C}$) of beam dose on a piece of Al foil. The results are displayed in Fig. 3-1.

The calibration is performed by the program VDGCAL.FOR [Bosh93c]. The resonance locations are hard-coded into the program. The calibration is performed using the linear relationship between the analyzing magnet field and NMR frequency,

$$B = s\omega + c, \quad (3-1)$$

where B is the magnetic field strength, ω is the NMR frequency, and s and c are the calibration slope and intercept respectively. Since we don't know B directly, we make use of

$$r = \frac{\sqrt{2mE}}{qB}, \quad (3-2)$$

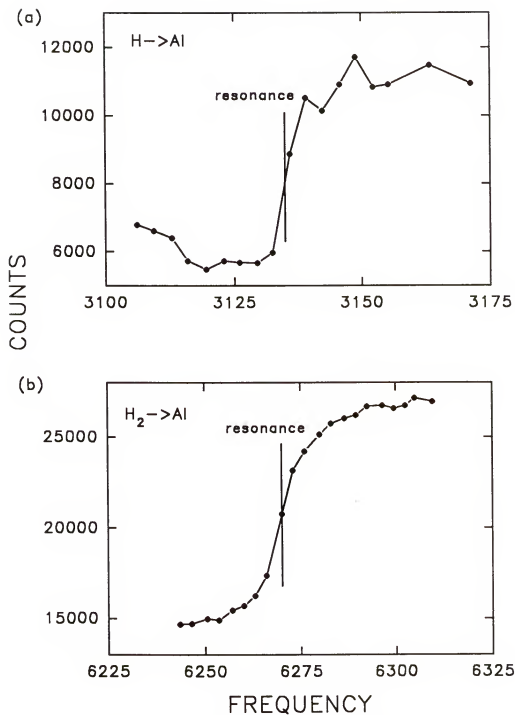


Figure 3-1. Total detected γ yield for a) H^+ and b) H_2^+ on Al as a function of the frequency of the NMR probe. The resonances are clearly evident, and allow calibration of the analyzing magnet as there is a linear relationship between frequency and magnetic field strength.

as r (radius of curvature for beam in the magnetic field), m (mass of projectile), and q (charge of projectile) are fixed, and we have measured E by the resonance location. We can now find the calibration slope and intercept using the two measured points (r and $\sqrt{2}$ have been absorbed into these parameters).

With the calibration in hand, the frequency setting for any desired beam is easily attained. VDGCAL.FOR will accept as input the mass and charge of a desired beam and will output the NMR frequency settings for a wide range of beam energies. The above calibration makes this procedure very simple,

$$\frac{\sqrt{m E}}{q} = s\omega + c. \quad (3-3)$$

One must keep in mind when setting the accelerating potential on the Van de Graaff that the charge of the desired beam determines the energy after acceleration,

$$E = qP, \quad (3-4)$$

where P is the Van de Graaff potential. However, most beams that will be produced will be singly charged, so this is not a concern. Indeed, the program actually takes the potential as input, and converts this to an energy based on the inputted charge. The output is also in the form of potential versus frequency.

Beam to Sample Alignment

High Vacuum Scattering

In this chapter, we will be dealing with a scattering chamber quite different than the UHV chamber discussed in Chapter 2 and used in later chapters. This second chamber is a high vacuum chamber, and the base pressure is 1×10^{-6} Torr. This is completely inadequate for surface studies, but our focus in this chapter is not on surface physics, but on ion channeling phenomena.

The features of this chamber are quite different than the UHV scattering chamber. The chamber itself is 10 inches in radius. The goniometer is equipped with two angular degrees of freedom similar to the UHV chamber. Angle A turns the goniometer so that the sample can be tilted with respect to the incident beam (about a vertical axis). Similarly, Angle C turns the goniometer about an axis normal to the goniometer surface. Angle B allows rotations about a horizontal axis (perpendicular to Angle C), but is not available on this goniometer. These angles are controlled by stepper motors (Motor A and Motor C) with a resolution of 0.02° . Translational motion perpendicular to the beam is possible in the vertical direction only. This allows more than one beam spot to be investigated, however, only about three beam spots are available on a single Si thin window with this limited motion. The Si surface barrier detector (solid angle 1.57 msr and in a horizontal plane containing the sample) is mounted on a rotatable plate in the bottom of the scattering chamber and allows virtually any scattering angle to be investigated with a resolution of better than 0.02° . Finally, the chamber is equipped with the usual collimation. An aperture 1.9 m up the beam line from the sample (1.6 mm in diameter) filters out most of the beam, while slits near the chamber entrance (0.4 m from the sample and about $0.5 \times 0.5 \text{ mm}^2$ in size) filter out beam scattered from the aperture and thus define the angular divergence of the beam. A beam spot on the sample of $0.8 \times 0.8 \text{ mm}^2$ with an angular divergence of 0.03° is achieved, with a typical beam current of 5 nA employed to minimize pulse pile-up in the detector.

AutoScan

The stepper motors are controlled by the program MOTORS.FOR [Dygo93a]. The stepper motors program and the Multi-Channel Analyzer program (MCA) were

interfaced by A. Dygo. This allowed automation of data collection. One indicates which (A,C) angles are desired (one can iterate over a single motor or input (A,C) pairs from a batch file), the stepper motors move there and data are collected by the MCA until a certain beam dose has been achieved. The stepper motors then move on to the next point, and the process is repeated.

This allows data such as that presented in Fig. 3-2 to be acquired with little effort. Here a Si(100) thin crystal has been placed in the scattering chamber so that the ion beam is roughly normal to the surface. The detector is located in a transmission geometry, and a window has been placed on the Si signal in MCA to monitor the Si counts. The sample was tilted by some arbitrary amount (8° in Motor A) so as to be tilted away from the $\langle 100 \rangle$ axis. The stepper motor/MCA interface (referred to as AutoScan from here on) was allowed to step by 1° in Motor C (azimuth), and MCA was allowed to collect for less than $1 \mu\text{C}$ at each step. This took several seconds per point, and the entire procedure can take an hour or more. AutoScan then plots Si counts versus Motor C, and we have Fig. 3-2. The dips in the Si yield correspond to the beam channeling along various planes in the Si crystal (some major planes are labeled in Fig. 3-2). We will return to this later.

Beam Direction Alignment

After AutoScan was properly working, the next task was to achieve beam-sample alignment. First, we needed to find the vertical translation of the sample holder and beam direction so that the beam would pass through the center of the sample holder. This was achieved with a small diameter (1 mm) thin window placed in the center of the sample holder. Both vertical translation (referred to as z) and the beam direction were varied until the beam passed through the small

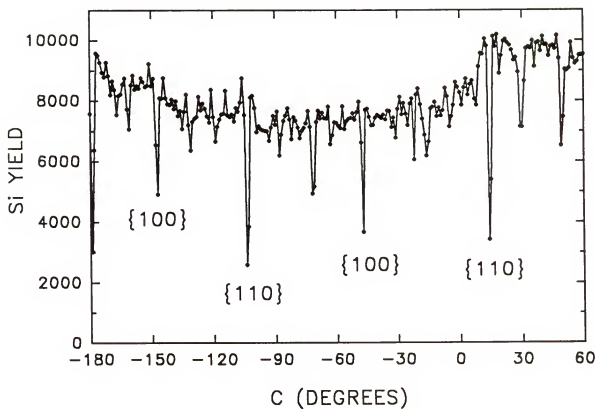


Figure 3-2. Silicon yield as a function of Motor C position, step size 1° . Motor A was fixed at 8° . The dips correspond to low-index planes in the Si crystal, and are used to calibrate the goniometer.

window. The beam direction was varied with the collimation and with the focusing quadrupole magnets and steering magnets. Once this was achieved, $z = 0$ was defined and the collimators were fixed. Since the exact beam direction varies from experiment to experiment, the beam is steered through the fixed collimators with the quadrupole and steering magnets, thus ensuring that the beam direction is not changed. In addition, by observing beam spot movement at large tilts, it was determined that the A axis did not quite pass through the sample. Washers were placed on the sample holder legs to correct this.

Goniometer Calibration and Coordinate Transformations

The rest of the beam-sample alignment procedure follows closely that described in Ref. [Dygo93c]. Important points in the procedure will be detailed here. We introduce the coordinates of the beam in the lab (goniometer) frame,

$$\vec{b} = \begin{bmatrix} b_x \\ b_y \\ b_z \end{bmatrix} = \begin{bmatrix} \sin \gamma \\ 0 \\ \cos \gamma \end{bmatrix}, \quad (3-5)$$

where γ represents a permanent misalignment between the beam and goniometer, and must be determined if the origin of B is to be determined accurately (see below). It can manifest itself if, for example, the goniometer arm is not perfectly vertical extending down into the scattering chamber. Using Eq. 3-5, and the Euler angles, the beam coordinates in the crystal frame can be written in the most general form as

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} b_x \cos B \cos C + b_z(-\cos A \sin B \cos C + \sin A \sin C) \\ -b_x \cos B \sin C + b_z(\cos A \sin B \sin C + \sin A \cos C) \\ b_x \sin B + b_z \cos A \cos B \end{bmatrix}. \quad (3-6)$$

Now we can solve for A, B, and C assuming that x, y, z, b_x , and b_z are known.

Since we cannot move Angle B, a permanent tilt of 5° about the A axis has been built into the goniometer so that the region for no solution for the above equations does

not coincide with the region near the sample normal (near our desired channeling directions).

Let us return for a moment to Fig. 3-2. As mentioned, the dips correspond to crystal planes. As these planes must all intersect in the $\langle 100 \rangle$ axis, a polar plot can be generated that will indicate where the $\langle 100 \rangle$ axis is located. If one plots the fixed Motor A position radially, and the Motor C position azimuthally on such a plot (see Fig. 3-3), and joins the planes, the planes should all intersect in a single point if the goniometer is properly calibrated. If the planes do not intersect in a single point, an iterative procedure which varies the origin of Angle A and Angle B is performed until the planes join. The amount that the A origin is off, A_r , can readily be taken care of by resetting the Motor A zero. B_r represents a permanent nonorthogonality as this angle cannot be moved. Note should be made of the fact that sometimes it can be difficult to decide exactly which planes to join together. Usually this is not a problem as the magnitude of planar dip between different planes can distinguish them (see Fig. 3-2). Also, two planes of the same type ($\{100\}$ and $\{110\}$ in Fig. 3-2) should intersect at a known angle, in this case $\sim 90^\circ$. After this procedure, we have the laboratory coordinates for several planes and an axis (intersection of the planes) for a calibrated goniometer.

We are now prepared to discuss transforming between arbitrary crystal coordinates (θ, ϕ) and lab angles (A,C). We need the cartesian coordinates for the axis unit vector and a planar unit vector obtained from the calibration procedure above (s_x, s_y, s_z) and (p_x, p_y, p_z) , respectively. This is straightforward as the angles A, B, and C for the directions are known for a calibrated goniometer, and we can use Eq. 3-6.

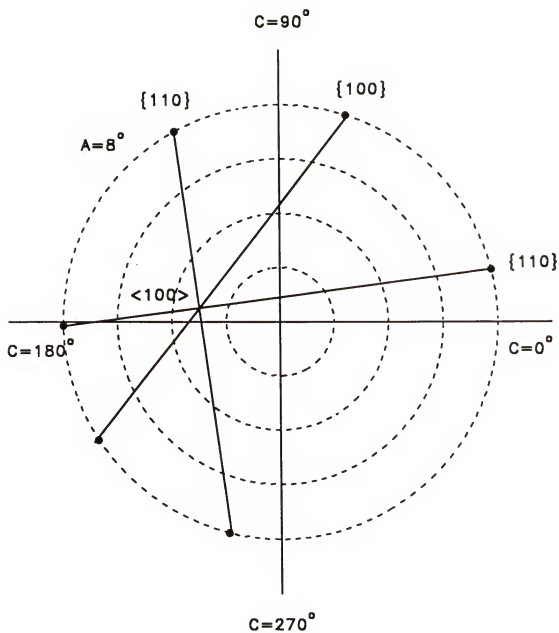


Figure 3-3. Polar plot (Motor A is the radial variable and Motor C is the azimuthal variable) showing the intersection in a single point of the planes found from Fig. 3-2. This indicates a well-calibrated goniometer. An iterative procedure can be used to locate the origin of Motor A (and B) if the planes do not intersect in a point.

The cartesian coordinates for any direction $\vec{r} = (x, y, z)$ can be obtained from the spherical coordinates (θ, ϕ) by

$$\vec{r} = \cos \theta \vec{s} + \sin \theta (\cos \phi \vec{t} + \sin \phi \vec{w}), \quad (3-7)$$

where $\vec{s}$ defines $\theta = 0$ (referred to as the reference string), $\vec{p}$ defines $\phi = 0$ (referred to as the reference plane), $\vec{t}$ is a unit vector along the perpendicular component of $\vec{p}$ with respect to $\vec{s}$, and $\vec{w} = \vec{s} \times \vec{t}$. Thus, if (θ, ϕ) is specified, we can obtain the cartesian coordinates using Eq. 3-7. Then, Eq. 3-6 can be solved to generate the lab angles (A,C). Alternatively, if (A,C) is specified, we readily obtain the cartesian coordinates with Eq. 3-6, and solve Eq. 3-7 to generate (θ, ϕ) .

Beam to Goniometer Misalignment and Sample Normal

The next alignment procedure that must be performed is to determine the beam-goniometer misalignment γ , alluded to above. This must be known in order to obtain B_r . This misalignment can be measured by tilting incrementally to large values for Motor A ($> 45^\circ$) and locating a nearly horizontal plane with Motor C. Realizing a horizontal plane requires some preparation in mounting the sample, but the sample cleaves along planar directions ($\{110\}$ for Si(100)), so this can be accomplished if the goniometer has been calibrated and properly zeroed. Figure 3-4 shows the results of this procedure. The plot is Motor C of the horizontal plane as a function of Motor A tilt. The solid dots are the experimentally determined planar positions. To obtain the expected planar coordinates, we must calibrate the goniometer as described above inputting a value for γ . We can then ask for the horizontal plane location for the tilts that we have investigated. Figure 3-4a shows the expected planar lab coordinates for $\gamma = 0.0^\circ$ (solid line) and $\gamma = 0.4^\circ$ (dashed line). Neither value produces a reasonable fit (and neither does any other

value). If small (0.3°) positional errors in the goniometer rotations are assumed (affecting the calibration procedure above), the experimental data can be fit quite well for $\gamma = 0.0^\circ$, and this value is assumed throughout this dissertation. This is shown in Fig. 3-4b.

Even though small positional errors were found in the goniometer, the reproducibility was found to be nearly perfect. To minimize the positional error, reference directions (an axis and a plane as described above) were only used if they were near (within a few degrees) of other directions being investigated. The alignment and transformation procedures described above are carried out by the program GON.FOR [Dygo93b].

The final alignment concerns the sample normal direction. This is found by locating the string, rotating the sample by 180° and locating the string again. The normal direction is the average of these two and is fixed.

Monte Carlo Simulation of Channeling and Data Reduction

The CXX channeling simulation code developed by A. Dygo has been well-documented in the literature [Dygo88; Dygo89; Dygo94c; Dygo94d]. The program C18.FOR [Dygo94a] is used to simulate channeling for crystal orientations close (up to 16° tilts) to the $\langle 100 \rangle$ axis. Similarly, the program C28.FOR [Dygo94a] is used for directions close to the $\langle 110 \rangle$ axis. In this section, the basics of the channeling simulation employed by the programs will be discussed. In addition, the extraction of energy distributions from the simulations will be covered, as well as the reduction of experimental data to compare with simulated energy distributions.

An overview of the simulation procedure is provided in Fig. 3-5. Both major axes are represented in this figure. An ion approaches near one of the two axes and

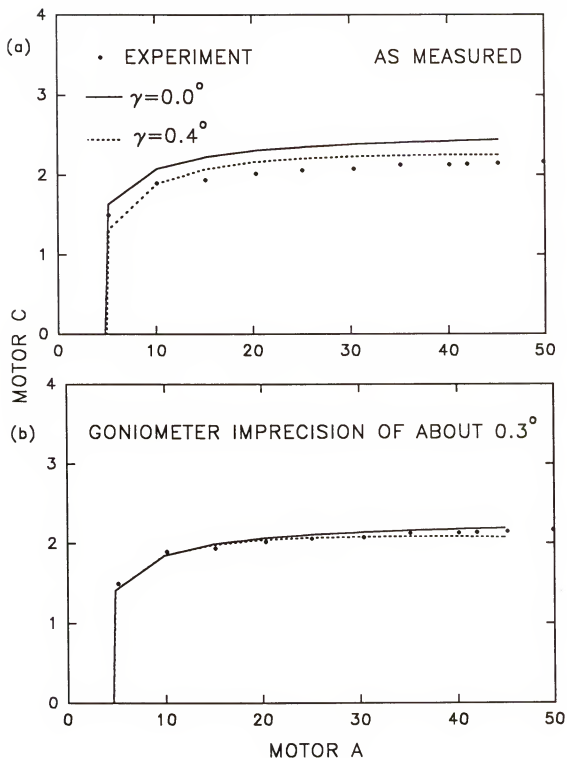


Figure 3-4. Determination of the beam-goniometer misalignment γ . The laboratory angles for a horizontal plane are measured for several large tilts (solid dots), and the expected location of the plane is plotted for $\gamma = 0.0^\circ$ and $\gamma = 0.4^\circ$ for a) as measured or b) assuming a small positional error in the goniometer; $\gamma = 0.0^\circ$ fits the data if a positional error is assumed.

sees a specific geometrical arrangement of Si atoms depending on the axial direction. The impact parameter (distance of closest approach) between the ion and a Si atom is calculated, and the ion is deflected from its path based on this impact parameter (its velocity is altered). Then the ion is followed along on a straight line until it approaches another Si atom, the impact parameter is calculated again, with a new deflection resulting. This process repeats throughout the Si crystal.

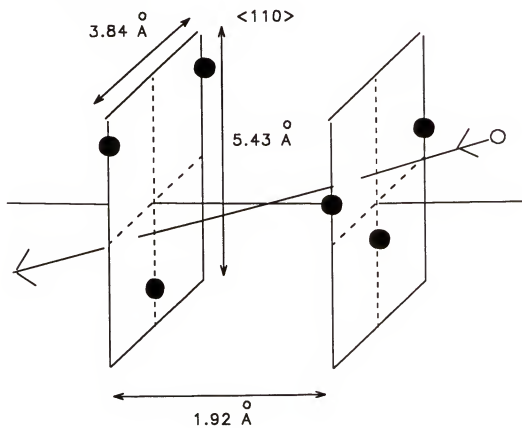
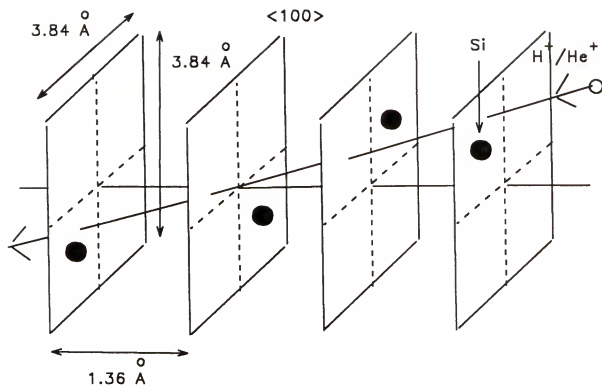
Interaction Zones

However, Fig. 3-5 is not how the actual calculation proceeds. First, we will consider the $\langle 100 \rangle$ axis. Figure 3-6 shows how the program operates for this axis. The black dots indicate Si atom rows, with the size of the dot showing proximity to the surface (the view is from above). The number of different sizes indicate the number of different types of atomic planes before repetition (in this case, four). The closest atom to the surface is located at the origin. To start the simulation, a random number is chosen between 0 and $\sqrt{2}$ for both x and y . This puts the incident ion in the upper right square (defined by the Si atom rows and marked START; a square such as this will be referred to as the basic channel as it is the smallest area that is repeated). The units used in the program are $4 \times$ fraction of a lattice constant ($1.92/5.43 \times 4 = \sqrt{2}$). The crystal orientation being simulated (θ, ϕ) is also specified, with ϕ being taken relative to the $\{100\}$ plane. This gives the ion velocity,

$$\vec{v} = \begin{bmatrix} v_x \\ v_y \\ v_z \end{bmatrix} = \begin{bmatrix} \sin \theta \cos \phi \\ \sin \theta \sin \phi \\ \cos \theta \end{bmatrix}. \quad (3-8)$$

The impact parameter between the ion and the origin is now calculated, and the velocity of the ion is altered based on the impact parameter. The ion is then followed on a straight line path as described, but on the next atomic plane, the Si

Figure 3-5. Overview of Monte Carlo simulation of channeling. The ion penetrates near one of two major axes in silicon, and the only difference in calculation between the two is the geometrical arrangement of Si atoms. The ion path is a straight line between atomic planes.



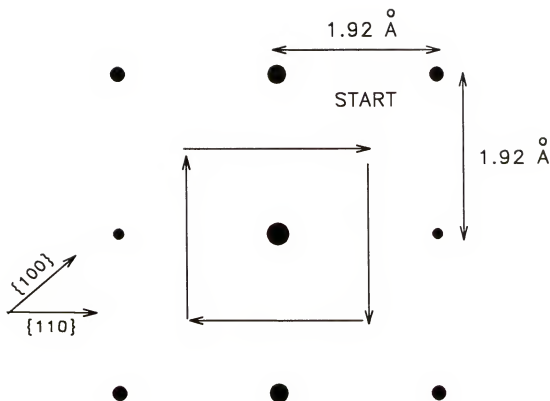


Figure 3-6. Interaction zone for directions near the $\langle 100 \rangle$ axis. The ion starts in the upper right basic channel, and the impact parameter is calculated with respect to the Si atom at the origin. Instead of varying this Si atomic position, the ion is moved according to the arrows for successive atomic planes. If an ion moves out of the interaction zone, it is moved back in by symmetry.

atom remains at the origin. The ion is moved to the bottom right basic channel (actually, the $\sqrt{2}$ is subtracted from the resulting y-coordinate of the ion, it doesn't necessarily have to reside in the bottom right channel). This is equivalent to changing the position of the Si atom (see Fig. 3-5 and below). The process repeats as shown in Fig. 3-6 by the arrows. If an ion leaves the region shown in Fig. 3-6, it is put back into the region by a shift which preserves the symmetry (the region in which the calculation proceeds, shown in the figure, will be referred to as the interaction zone). After the trajectory for an ion has been calculated for the entire crystal thickness, the calculation repeats for a new ion. Thus, a new random number is selected. The velocity will be the same (for now) as the simulation (involving thousands of incident ions) is for a single crystal orientation (θ, ϕ) .

Figure 3-7 shows the interaction zone for the $\langle 110 \rangle$ axis (the outlined rectangle defines the interaction zone and the basic channel). Both the interaction zone and basic channel are larger for this axis. For this axis as well, ϕ is relative to the $\{100\}$ plane. The two Si atom sizes indicate two atomic planes before repeating. The origin is in the center of the interaction zone.

There are three primary differences in calculation for this axis. First, the ion is randomly placed anywhere in the interaction zone ($-1 \leq x \leq 1$ and $-\sqrt{2} \leq y \leq \sqrt{2}$; the units are the same as for the previous case). Secondly, there are three Si atoms on a single atomic plane, located at $(0, \frac{-\sqrt{2}}{4})$ and $(\pm 1, \frac{\sqrt{2}}{4})$. These are the large dots in Fig. 3-7. The impact parameter for the ion from all three must be calculated, and a net deflection is used to change the ion's velocity. Finally, the ion is shifted back and forth along the arrows to simulate changing Si atom positions on successive atomic planes (if the ion is located in the bottom right rectangle defined

by the dotted lines, it will be moved to the top left for the next atomic plane by shifts in both x and y). Assuming an ion were located at the tail of the arrow, one can clearly see how this procedure works. Noting the distance to Si atoms in the next atomic plane (small dots), and moving the ion as the arrow shows, one can see that those distances now correspond to the large dots, and we have successfully simulated changing the atomic plane while not moving the Si atomic positions.

Impact Parameter and Ion Deflections

Now we consider some details in the calculations described above. First, one must calculate the impact parameter, $\vec{b}$. This procedure is outlined in Fig. 3-8, but is discussed in considerably more detail in Ref. [Dygo94d]. The atomic plane being considered is at $z = 0$, and the next atomic plane is at $z = d$. The ion's unit velocity vector is $\vec{v}$. The Si atom's equilibrium position is given by the large black dot. However, the Si atoms vibrate within the crystal. The vibrations are taken to be gaussian, with a standard deviation of $0.078 \text{ \AA}$. The Si atoms are allowed to vibrate in all three dimensions, giving the Si atomic position at $\vec{a}$. The atomic position is rapidly calculated by random sampling from a table that generates the proper gaussian distribution when scaled by the inputted standard deviation. The impact parameter, $\vec{b}$, is then readily calculated [Dygo94d]. Unless otherwise noted, from here on the impact parameter will refer to the magnitude of this vector, or the distance of closest approach.

The deflection function is obtained from a potential chosen for the ion-atom interaction. The potential used in the program is a Hartree-Fock ion-atom potential modified for solid state electronic densities [Dygo92; Smul92]. This potential was arrived at by testing various potentials against backscattering experiments in Si

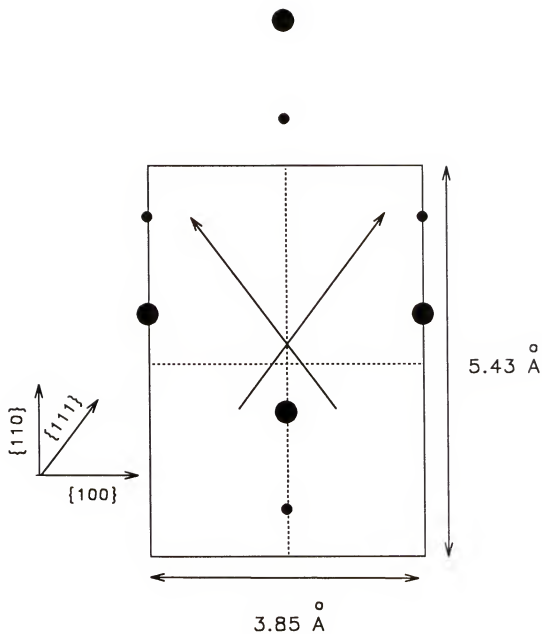


Figure 3-7. Interaction zone for directions close to the $\langle 110 \rangle$ axis. Three Si atoms reside on a single atomic plane, and all must be taken into account, so a net deflection is calculated. Again, the ion is shifted along the arrows so that the Si atom positions (large black dots) needn't be changed.

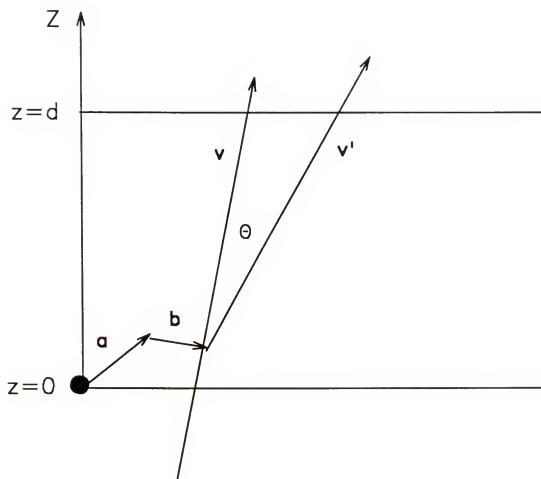


Figure 3-8. Calculation of impact parameter and $\vec{v}'$. The Si equilibrium position is the large black dot. The impact parameter is calculated assuming Si atomic vibrations in three dimensions, $\vec{a}$. The resulting deflection results in a new unit velocity vector which is followed to the next atomic plane $z = d$ where the calculation is repeated.

and $A^{III}B^V$ single crystals [Dygo89; Dygo90; Dygo92; Dygo94c; Dygo94d; Smul92]. The backscattering energy spectra show high sensitivity to details of ion trajectories, but are rather insensitive to the position dependence of the ion stopping power (thus, the ion stopping can be neglected in calculating the deflection function). However, the deflection function is energy dependent, so the deflections must be calculated based on an anticipated incident beam energy.

The resulting angular deflections for different impact parameters (.001 Å to .1 Å step size .0002 Å, and 0.1 Å to 1.7 Å step size .004 Å) are placed into a file which is read in by the Monte Carlo program. The effect is illustrated in Fig. 3-8. Based on the calculated impact parameter, the angular deflection is read from the table (linear interpolation is performed) and $\vec{v}^j$ results. This new velocity is followed to the next atomic plane $z = d$, and the entire process repeats. If b is less than .001 Å, corresponding to deflections larger than 9° , the ion is no longer followed (this occurs less than 0.5% of the time). If b is greater than 1.7 Å, deflections are negligible.

Additional Features

The program includes several other features as well, in an attempt to make the simulation as realistic as possible. The incident ion velocity is modified based on a gaussian distribution to take into account the experimentally determined angular beam divergence. Electronic multiple scattering is included as random gaussian deflections in the ion velocity with a standard deviation σ determined by Lindhard [Lind65] to be,

$$\sigma = \left(\frac{1}{2} \frac{m_e}{M_1} \frac{\Delta E}{E} \right)^{\frac{1}{2}}, \quad (3-9)$$

where M_1 is the ion mass, ΔE is the energy lost in a single ion-atom collision (see next section), and E is the ion energy. Surface layers (amorphous Si, C, O, etc.) can be included to simulate additional beam divergence.

Simulated Energy Distributions

The primary purpose (in this dissertation) for simulating channeling using the above program is to obtain the exit energy of the ions. In addition to constantly updating the trajectory of the ion, the program also keeps track of the energy lost by the ion as it penetrates the crystal and interacts with the Si host atoms. This is discussed in detail in the next section, but here the process for obtaining the proper output in the form of an energy distribution (distribution of final ion energies, after traversing the crystal and scattering into a detector). The idea will be to directly compare these energy distributions with experimental results, so a great deal of care is necessary in building the energy distribution from the ion exit energies.

It must first be noted that each ion that is simulated all the way through the crystal will be incorporated into the energy distribution as the experiments dealt with in this chapter will involve scattering from amorphous overlayers (this will be different in later chapters), so each ion will have an equal chance to scatter and be detected. Thus, when an ion completes its journey through the crystal, a count is added to an array element corresponding to the ion's energy. Typically 3200 to 6400 ion trajectories are followed. A normalized (unit area) counts versus energy spectrum is built up in this way, and this simulated spectrum is outputted.

Some corrections need to be taken into account, though. In order to make the corrections, the simulated spectrum is read in by the program E17S.FOR [Dygo94b]. To begin with, the number of counts in each array element needs to

be corrected since the Rutherford cross section depends on the energy of the ion before scattering (see Chapter 2). As the exit energy of channeled ions can vary, the number of counts in each array element is modified by

$$\text{counts} = \text{counts} \left(\frac{E_0}{E_{\text{exit}}} \right)^2, \quad (3-10)$$

where E_0 is the incident beam energy and E_{exit} is the energy associated with an array element. Energy straggling is also something that must be considered. Since straggling depends on the amount of energy lost (see Chapter 2), straggling corrections are also performed one array element at a time. That is, the energy of a single array element is considered. The corresponding amorphous Si thickness that the incident ions would have to penetrate to exit the crystal with this energy is calculated [Zieg77a; Zieg77b]. The straggling associated with this thickness is then determined [Yang91], and the array element is convolved by this amount. This process is repeated for all the elements in the array. The last correction made by E17S.FOR is to convolve the resulting spectrum for experimental resolution. This is determined by direct experiment and simulation comparison. This simulation and correction procedure is repeated for each crystal orientation investigated by experiment (the experimental resolution, FWHM, will be the same for all energy distributions once it is determined).

Experimental Energy Distributions

Having discussed generating simulated energy distributions, we now discuss generating their experimental counterparts. Table 3-1 shows a sample data reduction procedure. First, data are collected for several crystal orientations (θ, ϕ) , the same directions to be simulated. The procedure for converting between lab and crystal coordinates has been addressed. Both 625 keV H^+ and 2.5 MeV He^+ incident

beams are investigated (stopping is different, but velocity is the same). Scattering is from a thin (8 Å), amorphous gold layer (single isotope) on the beam-exit surface, and the detector is located in a transmission geometry at $\sim 80^\circ$. The experimental setup is outlined in Fig. 3-9. Note that the “random” direction (10,-10) where ϕ is relative to the {111} plane (this direction was identified by simulation, see later in this chapter) is repeated several times. This is to monitor the carbon buildup on both surfaces, which causes the spectrum to shift to lower energy with time as energy is lost by the beam in penetrating increasingly thicker carbon layers (this is not a concern under UHV conditions). Channeling degradation by increasing beam divergence in penetrating these layers was minimized by taking high symmetry directions first. The energy shift caused by the carbon layers is corrected for by calculating the (channel shift/ μC) between successive “random” spectra (the accumulated dose is carefully recorded). The several “random” spectra allow for nonlinearities in the carbon deposition rate ($\sim 10^{16} \text{Catoms}/(\text{cm}^2 \mu\text{C})$) to be accounted for.

The next step is to convert channel number to energy. The procedure for energy calibration of the detector has been discussed in Chapter 2. Here, we adjust the energy calibration somewhat to account for dividing out the kinematic factor for gold (we want the ion energy immediately after exiting the Si crystal, not after scattering from Au), as well as to address the shift to lower energies created by the carbon layers. If the energy calibration slope is slp , the intercept is int , the kinematic factor of Au at the experimental scattering angle is kf , and the calculated carbon shift is shift , we obtain the energy of a channel by

$$\text{energy} = \frac{\text{slp} \times \text{channel}}{\text{kf}} + \frac{\text{int}}{\text{kf}} + \frac{\text{shift} \times \text{slp}}{\text{kf}}. \quad (3-11)$$

Table 3-1. Sample data reduction procedure.

(θ, ϕ)	direction	dose	shift (channels)	$\cos \phi_{in}$	thickness ($\text{\AA}$)
(0,0)	$\langle 110 \rangle$	0.8	-26	.511	13910
(10,-10)	random	1.8	0.00	9.493	13888
(.2,0)		2.6	0.21	.325	13909
(.4,0)		3.4	0.41	.175	13909
(.6,0)		4.2	0.62	.188	13908
(.8,0)		5.0	0.83	.347	13908
(1,0)		5.8	1.03	.534	13907
(2,0)		6.6	1.24	1.520	13905
(10,-10)	random	7.6	1.50	9.493	13888
(10,0)	$\{111\}$	8.4	1.64	9.513	13889
(10,-.5)		9.2	1.78	9.511	13889
(10,-1)		10.0	1.93	9.510	13889
(10,-1.5)		10.8	2.07	9.509	13889
(10,-2.5)		11.6	2.21	9.506	13888
(10,-5)		12.4	2.35	9.501	13888
(10,-10)	random	13.2	2.50	9.493	13888
(10,36.25)		14.2	2.69	9.707	13897
(10,-54.74)		15.2	2.88	9.636	13894
(10,-44.74)		16.0	3.04	9.554	13890
(10,15)		16.8	3.19	9.572	13891
(0,0)	$\langle 110 \rangle$	17.6	3.35	.511	13910
(10,-10)	random	18.4	3.50	9.493	13888

Each spectrum will have a different shift due to accumulation of dose, as shown in Table 3-1. This process is carried out by the program EDN.FOR [Bosh94a], which also selects out the spectrum region corresponding to scattering from Au, and normalizes the entire set of spectra by a single normalization factor (which should be the case if the current integration is accurate, since we have an amorphous overlayer).

The simulated "random" energy distribution (an estimate is made for the Si thickness at this point) is now compared with one (usually the first taken) experimental "random" energy distribution. This serves several purposes. The normal-

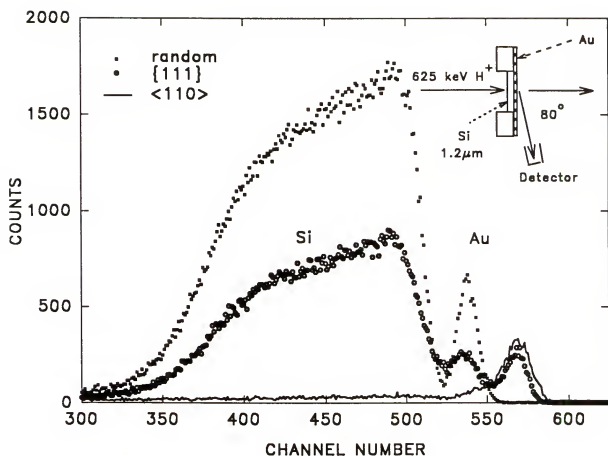


Figure 3-9. Energy spectra for 625 keV H ions transmitted through 1.2 μm thick Si crystal and scattered through 80°, taken in the random, aligned with the {111} planar, and aligned with the <110> axial directions.

ization factor used in EDN.FOR can be adjusted, and the experimental FWHM can be varied until an optimum fit is obtained. These values are then fixed for all other distributions. Further, the exact Si crystal thickness to be input into the simulation program can be fine tuned by shifting the simulation with respect to the data, and recording the number of keV that were added or subtracted to obtain a fit. The thickness correction can then be estimated by noting the number of Å's necessary (on average) for the ion to lose 1 keV of energy (easily done for “random” directions). The resulting crystal thickness is for the beam aligned with the “random” direction. To obtain the crystal thickness for the other directions, we use

$$\text{thickness} = \left(\frac{\cos \theta}{\cos \phi_{\text{in}}} \right) \text{norm thickness}, \quad (3-12)$$

where θ is the usual sample tilt, $\cos \phi_{\text{in}}$ is the dot product of the Si normal direction and the beam direction (obtained using GON.FOR), and norm thickness is the thickness along the Si normal direction (obtained from the “random” thickness using Eq. 3-12 in reverse). These small path length corrections are also illustrated in Table 3-1, and generate the Si crystal thicknesses that will be input into the Monte Carlo simulation for the respective crystal orientations.

Energy Loss Models

We make the usual assumption that core and valence electrons contribute independently to the stopping [Gemm74]. The interaction of the ion with valence electrons is treated within the free-electron gas (FEG) theory [Appl67]. The energy losses to valence electrons are divided into the contribution due to single-particle excitations that occur in close collisions, and the contribution due to collective (plasma) excitations that occur through distant collisions. The first contribution is

assumed to be proportional to the local valence electron density, while the second one is taken proportional to the average valence electron density. The energy lost by the ion (to core and valence electrons) in an individual collision with the lattice atom, for an impact parameter b , can thus be written as

$$\Delta E_a(b) = \Delta E_c(b) + \Delta E_{v1}(b), \quad (3-13)$$

where ΔE_c represents the energy loss to core electrons, and ΔE_{v1} is the energy lost in close collisions with valence electrons of the atom. The energy loss due to collective excitations of the valence electron gas, not being associated with any particular ion-atom collision, does not enter into Eq. 3-13. Instead, it is figured in based on the total path length of the ion between atomic planes.

When the impact-parameter dependent energy loss is integrated over all b 's, one gets the respective stopping cross section, for instance

$$\epsilon_c = \int_0^{\infty} \Delta E_c(b) 2\pi b db. \quad (3-14)$$

Similarly, ϵ_{v1} and $\epsilon_a = \epsilon_c + \epsilon_{v1}$ are obtained by integrating ΔE_{v1} and ΔE_a , respectively. It is convenient to normalize the above energy losses by their corresponding stopping cross sections, which defines functions of b referred to as $L(b)$. For example:

$$L_c(b) = \frac{\Delta E_c(b)}{\epsilon_c}. \quad (3-15)$$

Within the restricted energy interval considered here, the dependence of the functions L on the energy (velocity) of the ion can be neglected. Obviously, they satisfy the normalization condition

$$\int_0^{\infty} L(b) 2\pi b db = 1. \quad (3-16)$$

The total (random) stopping cross section is given by

$$\epsilon_r = \epsilon_a + \epsilon_{v2} = \epsilon_c + \epsilon_{v1} + \epsilon_{v2}, \quad (3-17)$$

where ϵ_{v2} is the contribution due to distant collisions with the valence electron gas (plasmon excitation). In the calculations to be presented, ϵ_r is taken from the semi-empirical tables of Ref. [Zieg77a].

Three-Component Model

Let us consider a specific example. We can consider a model in which the stopping due to core electrons is due entirely to close collisions. Such stopping is again taken to be proportional to the density of core electrons that the ion encounters,

$$L_c(b) = \frac{1}{Z_c} \int_{-\infty}^{+\infty} n_c(\vec{r}) dz. \quad (3-18)$$

Z_c denotes the number of core electrons per atom, and $n_c(\vec{r})$ is the core electron density (associated with a single atom). The integral is taken along the ion's trajectory (as it passes the atom) which is approximated by a straight line ($r^2 = b^2 + z^2$). Based on the SCA calculations (see below), the contribution of K-shell electrons to the stopping of 625 keV H ions can be neglected. Therefore, only L-shell electrons are included when evaluating Eq. 3-18. Their density is determined based on the Roothaan-Hartree-Fock (RHF) atomic wave functions [Clem74]. The evaluation of Eq. 3-18 is performed for 2000 impact parameters (.0005 Å to 1.9995 Å, step size .001 Å), and stored in a file for input by the Monte Carlo program (where linear interpolation is performed for arbitrary b). If b is greater than 2 Å, $L(b)$ is negligible.

From Eq. 3-15, we see that now we only need ϵ_c in order to be able to evaluate the energy loss from close collisions with core electrons, since we have calculated

L(b). This is readily obtained from Eq. 3-17, since ϵ_{v1} and ϵ_{v2} are easily calculated (see later). Thus, when an impact parameter is evaluated in the course of the channeling simulation, the energy of the ion is reduced based on the calculations discussed here. The stopping due to valence electrons is evaluated in an analogous manner (see later).

Figure 3-10 shows how this model stands up to experiment [Dygo94e]. Several crystal orientations were investigated for 625 keV H^+ ions incident on Si single crystal (thickness $0.57 \mu m$). See Fig. 3-9 for the scattering geometry and sample raw energy spectra. The data reduction was performed as described previously. The dots are the experimental energy distributions. The dashed lines represent the three-component energy loss model described here. The solid lines incorporate distant collisions with core electrons using the mean excitation energy approximation described below. Clearly, distant collisions with core electrons are necessary to accurately simulate the stopping.

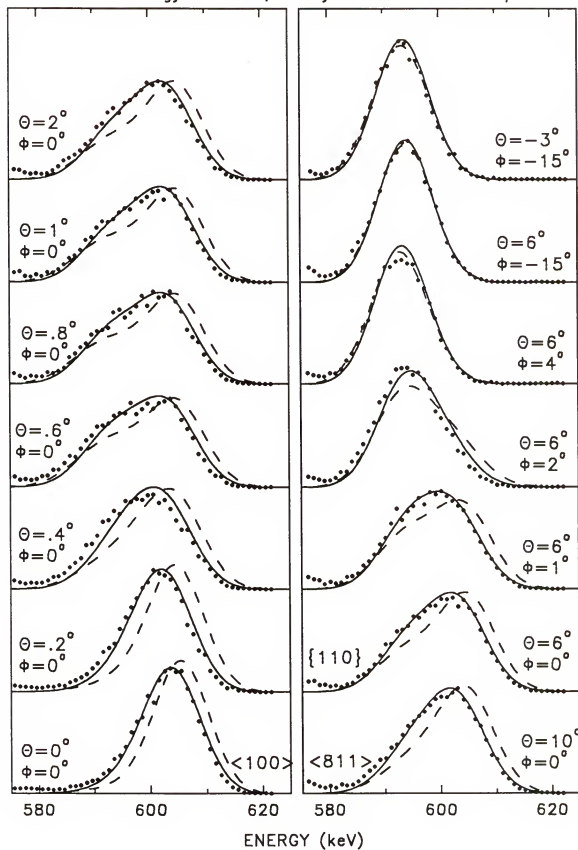
The reason that this model is not sufficient is that most ions maintain large impact parameters from the Si atoms. The primary interaction with core electrons is through distant collisions. Ignoring distant collisions with core electrons causes the severe underestimation in the stopping observed in Fig. 3-10. We must attempt to include distant collisions with core electrons if we hope to attain agreement between theory and experiment.

Semi-Classical Approximation

The energy loss due to core electrons is calculated within first-order perturbation theory using the semi-classical approximation (SCA) method of Kabachnik *et al.* [Kaba88]. The method involves an explicit summation of all contributions due

Figure 3-10. Experimental (dots) and Monte Carlo simulated energy distributions for the three-component model (dashed lines) and a model incorporating distant collisions with core electrons (solid lines).

H beam energy 625 keV, Si crystal thickness $0.57\mu\text{m}$



to excitation and ionization of the atom which is described by the Hartree-Slater approximation. The SCA model was successfully applied to explain data on the angular dependence of the energy loss in thin films [Bala88; Kaba92]. In contrast to channeling experiments, these data are most sensitive to small impact parameters. The model was also used in a number of studies on energy loss of channeled protons and antiprotons [Bala90a; Bala90b; Trik92]. Recently, a good agreement with the SCA model predictions was found by Auth and Winter in a study of the energy loss of 100 keV protons in single collisions with Ar atoms [Auth93]. Additionally, the calculation of the impact-parameter dependent straggling within SCA agreed very well with experimental data [Kaba93].

The L_c function for a 625 keV H ion on a Si core, calculated within the SCA model, is plotted in Fig. 3-11. In this calculation, the energy loss due to excitation to bound states is neglected, as it is estimated to contribute about 5% to the total energy loss. The calculation indicates that K-shell electrons give a significant contribution to the energy loss at very small impact parameters only (about 16% for $b = 0$, and rapidly vanishing by $b = 0.1 \text{ \AA}$). One can conclude, therefore, that the K-shell electron contribution to the stopping cross section is negligible (Eq. 3-14).

The SCA model was incorporated into the Monte Carlo program in the following way. The energy loss for 625 keV protons in Si due to the core electrons for various impact parameters was calculated by Kabachnik and sent to us. A program, KABACH.FOR [Bosh94b], was then employed to perform linear interpolation of these results for the 2000 b 's used by the Monte Carlo program, and the results were output to a file. This file was then directly used by the Monte Carlo program as usual. Since there is no reason to expect that Eq. 3-17 will be automatically

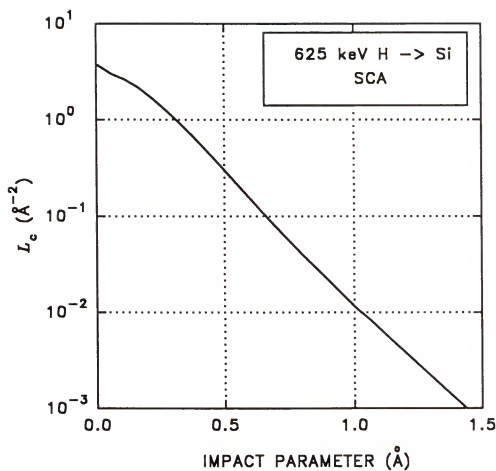


Figure 3-11. L_c function for 625 keV H ion on a Si core calculated within the SCA model.

satisfied from these calculations, these results will have to scaled somewhat depending on the valence electron contributions to the stopping. Scaling up by a few percent can be expected since excitations to bound states have been neglected.

Mean Excitation Energy Approximation

As an alternative approach, we divide the core electron contribution to the stopping (ϵ_c) into a close collision part (ϵ_{c1}) and a distant collision part (ϵ_{c2}) (4-component model). Assuming the equipartition rule [Lind64] we have $\epsilon_{c1} = \epsilon_{c2}$. The position-dependent stopping cross section related to close collisions is assumed to be proportional to the local density of core electrons, while the energy loss due to distant collisions is calculated within the dipole approximation with the mean excitation energy. Hence, the energy loss due to close collisions with core electrons is given by $\Delta E_{c1} = \epsilon_{c1} L_{c1}(b)$, where $L_{c1}(b)$ is calculated according to Eq. 3-18.

To calculate the distant collision term, L_{c2} , the dipole approximation as discussed by Beloshitsky and Kumakhov [Belo78; Kuma81] is used. Assuming a mean electronic excitation energy $\hbar\omega_j$ for a shell j , the energy transferred to a single electron l can be written as

$$\Delta E_{lj}(b) = \frac{2Z_1^2 e^4}{m_e v^2 b_j^2} \Omega_j^2 \left[K_0^2(\Omega_j \frac{b}{b_j}) + K_1^2(\Omega_j \frac{b}{b_j}) \right], \quad (3-19)$$

where Z_1 is the projectile atomic number, e is the electron charge, m_e is the electron mass, v is the projectile velocity, $\Omega_j = \omega_j/\omega_{j\infty}$ is the mean excitation energy ($\hbar\omega_j$) measured relative to the binding energy ($\hbar\omega_{j\infty}$), $b_j = v/\omega_{j\infty}$, and K_0 and K_1 are the modified Bessel functions. Again, Eq. 3-19 is applied to the L I, L II, and L III shells only. (Their respective binding energies are 149.7 eV, 99.8 eV, and 99.2 eV [Lide92].) By summing over all electrons in inner shells, one thus gets $\Delta E_{c2}(b) = \sum_j \sum_l \Delta E_{lj}(b)$, and $L_{c2}(b) = \Delta E_{c2}(b)/\epsilon_{c2}$. However, Eq. 3-19 is derived

for impact parameters greater than the shell radius, and it diverges for $b \rightarrow 0$. In order to evaluate L_{c2} for small b , a third-order polynomial form was assumed: $L_{c2}(b) = c_0 + c_1 b + c_2 b^2 + c_3 b^3$. The cutoff value of the impact parameter, b_c , where the two branches meet, and the parameters c_i ($i = 0, \dots, 3$) were uniquely determined by requiring that (1) the derivative of L_{c2} at $b = 0$ vanishes, (2) both the L_{c2} and its derivative at $b = b_c$ for the two branches are equal to each other, (3) Eq. 3-16 is fulfilled, and (4) L_{c2} monotonically decreases between 0 and b_c , and the difference between $L_{c2}(0)$ and $L_{c2}(b_c)$ is as small as possible. For example, if one assumes $\Omega_j = 1$, the resulting b_c (for 625 keV H on Si) is 0.64 Å, while for $\Omega_j = 1.4$ one gets $b_c = 0.46$ Å.

The L_c functions (i.e. $\frac{1}{2}L_{c1} + \frac{1}{2}L_{c2}$), calculated within the mean excitation energy approximation (MEEA) for three values of the parameter Ω (1, 1.2, and 1.4), are compared with the SCA dependence in Fig. 3-12. While $\Omega = 1$ clearly overestimates the energy loss for large impact parameters ($b > 0.5$ Å), the curve for $\Omega = 1.4$ is remarkably close to the SCA prediction in the whole range of impact parameters. Let us note that within the MEEA model, $\Delta E_{c2}(b)$ (for $b > b_c$) and ϵ_{c2} are independent of each other, so the resulting L_{c2} function depends on the chosen value of ϵ_{c2} . The latter, in turn, is related to ϵ_v ($= \epsilon_{v1} + \epsilon_{v2}$) through the equation $\epsilon_{c2} = \frac{1}{2}(\epsilon_r - \epsilon_v)$, where the random stopping cross section, ϵ_r , is a fixed quantity (for a given energy). The value of ϵ_v is determined by the parameter β , defined below. The results presented in Fig. 3-12 were calculated for $\beta = 0.94$. This value corresponds to the best fit to the experimental energy distributions, obtained using the SCA model (see below).

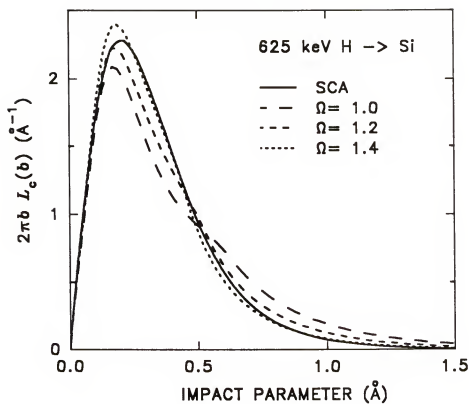


Figure 3-12. $2\pi b L_c$ functions calculated within the MEEA model for three values of Ω (and $\beta = 0.94$), compared with the SCA calculation.

The parameters b_c and c_i were found by the program LKUM.FOR [Bosh94h]. First, ϵ_{c2} is found as described. Then, Eq. 3-19 is evaluated for core electrons, and $L_{c2}(b)$ is obtained via Eq. 3-15. A trial b_c is now chosen, and $L_{c2}(b)$ and its derivative at b_c are evaluated (FUNCT and DERIV, respectively).

Condition (i) yields $c_1 = 0$. Condition (ii) yields $c_2 = \frac{3 \text{FUNCT} - \text{DERIV } b_c - 3 c_0}{b_c^2}$ and $c_3 = \frac{\text{DERIV } b_c - 2 \text{FUNCT} + 2 c_0}{b_c^3}$. Next, c_0 is varied so that Eq. 3-16, condition (iii), is satisfied. Finally, condition (iv) is met by varying b_c itself. The parameters for $\Omega_j = 1.4$, the model that best reproduces the SCA model, are $b_c = 0.46 \text{ \AA}$, $c_0 = 1.1847$, $c_1 = 0$, $c_2 = 0.2220$, and $c_3 = -6.8265$.

Valence Electrons

As mentioned earlier, the valence electron contribution to the stopping is treated within the free electron gas theory. The stopping cross sections due to close and distant collisions are calculated according to the formulae [Appl67]:

$$\epsilon_{v1} = \beta \frac{4\pi Z_1^2 e^4}{m_e v^2} Z_v \ln \frac{2m_e v v_F}{\hbar \omega_p} \quad (3-20)$$

and

$$\epsilon_{v2} = \beta \frac{4\pi Z_1^2 e^4}{m_e v^2} Z_v \ln \frac{v}{v_F}, \quad (3-21)$$

where Z_v is the number of valence electrons per atom and β is introduced here as a scaling parameter. In the above formulae the Fermi velocity v_F and the plasmon energy $\hbar \omega_p$ are calculated for the average density of valence electrons in the crystal.

Based on the assumption that the position-dependent stopping due to close collisions is proportional to the local density of valence electrons, one gets the formula for L_{v1} that is analogous to Eq. 3-18 for the core electron term L_{c1} (obtaining L_{v2} is trivial since the average valence electron density is used). However, the valence electron density (associated with a given atom) extends to much larger distances than

the core electron density does. More importantly, due to the directional bonding effects, the valence electron density in solid Si is not isotropic. Thus, in general, the L_{v1} function depends on the impact parameter vector $\vec{b}$ rather than on its absolute value b . Therefore, from a programming point of view, it is convenient to calculate a 2-dimensional map $L_{v1}(\vec{b})$ across the channel, to be used in the simulation code. The $L_{v1}(\vec{b})$ map is no longer associated with a single atom but includes contributions from all atoms that are sufficiently close to a given point within the channel area. Consequently, the argument $\vec{b}$ ceases to be an impact parameter with respect to any particular atom. Instead, it is a 2-component position vector with respect to a chosen frame of reference. The use of $L_{v1}(\vec{b})$ map simplifies and speeds up the simulations, but it is strictly valid only for trajectories parallel to the axis along which the electron density is integrated. For trajectories tilted by ψ with respect to the axis, the energy loss is approximated by $\epsilon_{v1} L_{v1}(\vec{b}) / \cos \psi$.

Maps of $L_{v1}(\vec{b})$ were tabulated for both solid-state and free-atom valence electron densities with a resolution of $0.0543 \text{ \AA}$ (along the $\{110\}$ plane) $\times 0.0384 \text{ \AA}$ (along the $\{100\}$ plane) for the $\langle 110 \rangle$ axis, and a resolution of $0.0384 \text{ \AA} \times 0.0384 \text{ \AA}$ (along the $\{110\}$ planes) for the $\langle 100 \rangle$ axis. The solid-state electron density was taken from the analysis of x-ray diffraction measurements by Deutsch [Deut92], while the free-atom electron density was based on the RHF wave functions [Clem74]. Both maps consider contributions to the density from all atoms (on a given atomic plane) within a distance of about $4 \text{ \AA}$. The 2-D maps were obtained by generation of the valence electron density in the Si unit cell (using the results of the references), and integrating the density corresponding to the axial direction desired.

The L_{v1} functions corresponding to the solid-state and free-atom valence electron densities are compared in Figs. 3-13 and 3-14. In order to reflect the symmetry of the channel, the values plotted include contributions of 2 successive planes for the $\langle 110 \rangle$ axis and 4 successive planes for the $\langle 100 \rangle$ axis. Figure 3-13 shows the values of L_{v1} in the case of the $\langle 110 \rangle$ axis, calculated across the channel and along the bond, as indicated in the insets. The dotted line corresponds to the average density of valence electrons. The two densities produce quite similar results, except for the mid-bond region where the solid-state curve exceeds the free-atom values by 25%. Both densities predict a substantial reduction of L_{v1} in the middle of the $\langle 110 \rangle$ channel. In the case of the solid-state density, the minimum value of L_{v1} amounts to 21% of the average value. The results obtained in the case of the $\langle 100 \rangle$ axis are shown in Fig. 3-14. Let us note that "along bond" means here: along the projection of the bond. The differences between the L_{v1} functions corresponding to the solid-state and free-atom densities are even smaller in this case. Surprisingly, the absolute minimum of L_{v1} across the channel and along the bond is found at a distance of about $0.3 \text{ \AA}$ from the atom rows, and not at the center of the channel. Thus, the minimum energy loss observed in the case of the $\langle 100 \rangle$ axial channeling is in fact due to the impact-parameter dependence of the energy loss to core electrons (see Fig. 3-11), which overcompensates the valence electron term shown in Fig. 3-14.

The above approach to the position-dependent valence electron stopping, which assumes the contribution due to close collisions to be proportional to the local valence electron density, while the contribution due to distant collisions is taken proportional to the average density of valence electrons, will be referred to as the

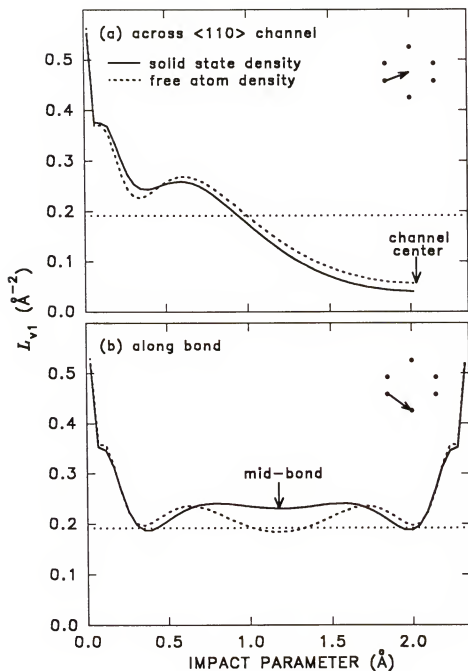


Figure 3-13. L_{v1} functions for the solid-state and free-atom valence electron densities for the $\langle 110 \rangle$ axis in Si (a) across the channel and (b) along the bond, as indicated in the insets.

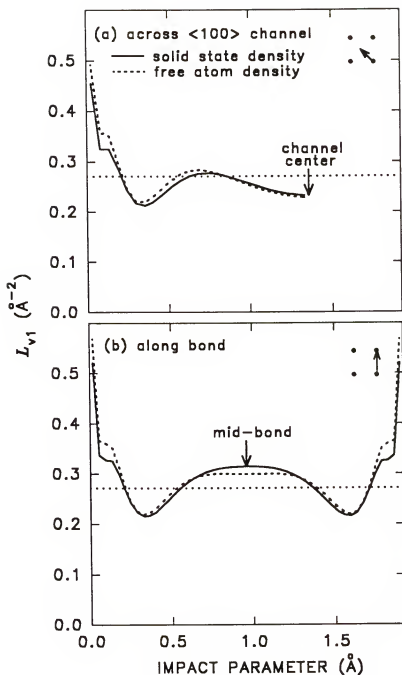


Figure 3-14. L_{v1} functions for the solid-state and free-atom valence electron densities for the $\langle 100 \rangle$ axis in Si (a) across the channel and (b) along the projection of the bond, as indicated in the insets.

2-component FEG model. In addition, to investigate sensitivity of the energy distributions to various assumptions about the valence electron stopping, two limiting cases are considered. First, the non-uniformity of the valence electron gas is disregarded, i.e. the total energy loss to valence electrons is made proportional to their average density. This approach will be referred to as the constant density model. Second, the contributions due to both close and distant collisions are assumed to be proportional to the local density of valence electrons. Then the total energy loss to valence electrons is given by $\Delta E_v(\vec{b}) = \epsilon_v L_{v1}(\vec{b})$, where $\epsilon_v = \epsilon_{v1} + \epsilon_{v2}$. Based on Eqs. 3-20 and 3-21, one obtains

$$\epsilon_v = \beta \frac{4\pi Z_1^2 e^4}{m_e v^2} Z_v \ln \frac{2m_e v^2}{\hbar \omega_p}. \quad (3-22)$$

At our projectile velocity ($v/v_F \approx 5$) the above expression agrees to within 0.5% with the results given by Lindhard and Winther [Lind64], if the local value of ω_p is used. Although in our calculations the plasma frequency corresponding to the average valence electron density has been used, it only has a minor effect on the results, as ω_p enters in Eq. 3-22 through the logarithm. Therefore this approach will be referred to as the Lindhard-Winther (LW) model.

H⁺ Near the $\langle 100 \rangle$ and $\langle 110 \rangle$ Axes

In this section, energy-loss distributions for 625 keV H⁺ ions in thin Si single crystals are studied as a function of the crystal orientation (based on our paper Ref. [Dygo94f]). Detailed angular scans are taken through the $\langle 110 \rangle$ and $\langle 100 \rangle$ axes as well as through the most open planar channels intersecting these axial directions, i.e. the $\{111\}$ and $\{110\}$ planes, respectively. The experimental distributions are very well reproduced by a Monte Carlo simulation using the semi-classical approximation (SCA) of Kabachnik *et al.* [Kaba88] to describe the energy loss to core

electrons, and the free electron gas (FEG) model to determine the energy loss to valence electrons. It is found that the mean excitation energy approximation, used to calculate the impact-parameter dependence of the core electron contribution to the stopping in our preliminary report [Dygo94e], can reproduce the SCA results quite well. Various approaches to the valence electron contribution are also analyzed: the Lindhard-Winther local density approximation [Lind64] versus constant density approximation, as well as the use of the solid-state versus free-atom electron densities. Based on individual ion trajectories and ion flux distribution calculations, the evolution of the energy distributions as a function of tilt angle with respect to the axial direction is discussed. Also, random-like directions near the $\langle 110 \rangle$ axis are identified by means of a detailed study of the orientation dependence of the mean energy loss.

Experiment

Two separate experiments were performed to measure the energy distributions for directions near the $\langle 110 \rangle$ and $\langle 100 \rangle$ axes, using two different Si single crystals. As the equipment and procedures used in the two experiments were essentially the same, we will confine ourselves here to the $\langle 110 \rangle$ experiment.

The incident beam of H^+ ions, produced and accelerated to 625 keV by the UF 3.5 MV Van de Graaff, was collimated to a cross-sectional area of $0.8 \times 0.8 \text{ mm}^2$ and an angular divergence of 0.03° . A $1.2 \text{ }\mu\text{m}$ thick Si(110) sample was prepared using a dopant-selective etching technique [Seib93], and a $10 \text{ }\text{\AA}$ thick amorphous layer of Au was deposited on the 10% HF-dipped surface. The etched area of the sample had a diameter of 5 mm, with a thickness variation of 5–10%. The sample was mounted on a two-axis goniometer, stepper motor driven with a resolution of 0.02° .

The goniometer was also equipped with translation perpendicular to the beam. The ions scattered through 80° were detected in a transmission geometry (the Au layer on the beam exit side, as shown in Fig. 3-9), and energy-analyzed using a Si surface-barrier detector with an acceptance angle of 2.5° . The base pressure in the scattering chamber was 5×10^{-6} Torr.

The scattering yield from Si was used to align planar and axial directions to the beam. The goniometer-beam system was calibrated, and the alignment for any direction in the crystal was achieved to a precision of 0.02° – 0.05° by applying the methodology developed in Ref. [Dygo93c]. Both the multi-channel analyzer and the stepper motors on the goniometer were controlled by a personal computer. Once reference directions were established (usually an axial and a planar direction), the energy distributions corresponding to full angular scans in the crystal coordinates, involving rotations about both axes of the goniometer, were taken in a completely automated way.

The energy distributions of the H ions transmitted through the Si single crystal were retrieved from the Au signal by dividing the measured energy by the kinematic factor. A total of 21 distributions were taken on the same target spot to assure no variation in sample thickness. Each distribution was collected for $0.8 \mu\text{C}$ of the integrated beam charge. Two angular scans were performed: (1) through the $\langle 110 \rangle$ axis along the $\{111\}$ plane, and (2) perpendicular to the $\{111\}$ plane at a tilt $\theta = 10^\circ$ with respect to the $\langle 110 \rangle$ axis. The tilts included in the scan (1) were: $\theta = 0^\circ$ (i.e. the $\langle 110 \rangle$ axis), 0.2° , 0.4° , 0.6° , 0.8° , 1° , and 2° , while the azimuthal angles studied in the scan (2) were: $\phi = 0^\circ$ (i.e. the $\{111\}$ plane), 0.5° , 1° , 1.5° , 2.5° , 5° , and 10° ($\phi = 54.74^\circ$ corresponds to the $\{100\}$ plane, while $\phi = -35.26^\circ$ corresponds to the

$\{110\}$ plane). Based on our simulation results presented below, the tilt of 10° is large enough to avoid the influence of the $\langle 110 \rangle$ axis. The direction $(\theta, \phi) = (10^\circ, 0^\circ)$ can thus be considered to represent a “pure” $\{111\}$ plane. It will be further shown that the mean energy loss for the direction $(\theta, \phi) = (10^\circ, 10^\circ)$ approximates the random value to better than 1%.

As a consistency check, a number of random-like distributions (for specific directions) were taken, followed by a repeated measurement of the $\langle 110 \rangle$ distribution. Comparison between the two measurements for the $\langle 110 \rangle$ direction revealed a slight change in the shape of the distribution as well as a shift toward lower energies. These changes are primarily due to carbon deposition on both sides of the sample during the irradiation. Changes in the distribution can also result from structural defects in the sample, introduced by the irradiation. However, as the distributions for the most sensitive directions (close to the $\langle 110 \rangle$ axis) were taken at the beginning of the measurement sequence, they do not seem likely to be affected by significant radiation damage. In order to determine the amount of the shift due to the carbon layers, the distributions for the direction $(\theta, \phi) = (10^\circ, 10^\circ)$ were taken at the beginning of each scan (in addition to the measurement at the end of scan (2)), as well as at the end of the whole sequence. The magnitude of the shift for all other distributions was determined by linear interpolation based on the accumulated beam dose, and the distributions were corrected accordingly. The estimated shift corresponded to about 10^{16} C atoms/cm²/μC deposited on both sides of the sample.

The sample thickness, the normalization constant for all distributions, as well as overall energy resolution were determined based on the distribution for the direction $(\theta, \phi) = (10^\circ, 10^\circ)$, by requiring that the simulated distribution (see next section)

matches the experiment. The distributions for random-like directions depend on the random value of the stopping cross section assumed in the simulation, but are insensitive to the impact-parameter dependence of the energy loss. As the random stopping cross section is known in our energy range to an accuracy better than 5%, the same (in)accuracy is achieved in the thickness determination. This does not affect the energy distributions because for a sample about $1\text{ }\mu\text{m}$ thick, the ion flux distribution (and, consequently, the energy distribution if normalized to the random energy loss) does not change significantly if the thickness is increased (decreased) by 5%. The overall energy resolution was found to be 10 keV. This value includes the detection system resolution, the energy spread of the incident beam, and the effect of the sample nonuniformity.

A final note concerns the overlap of the Si and Au signals seen in Fig. 3-9. The Si signal consists in fact of two components: one that is due to scattering within the single-crystalline material, and the other one coming from scattering by the amorphous oxide layer at the Au/Si interface. The latter registers the energy distribution of the transmitted ions in the same way as the Au signal does. However, it appears shifted to lower energies and is much weaker than the Au signal, due to the smaller kinematic factor and scattering cross section of Si, as well as the smaller thickness of the oxide. It can be estimated that the shift amounts to 29 keV for the $\langle 110 \rangle$ direction, and 27 keV for the random direction (see the energy distributions presented below).

Results and Discussion

Energy Distributions. Seeking to reproduce the experimental energy distributions, we will use the SCA model to determine the impact-parameter dependence of

the energy loss to core electrons. The MEEA model only serves as a simple approximation to the more accurate SCA calculation and will be used later on to test the sensitivity of the energy distributions to the core electron contribution to $\Delta E(b)$. In order to investigate the influence of the valence electron term on the distributions, we first consider the three approaches to the valence electron stopping, discussed previously. The stopping cross sections due to valence electrons are calculated from Eqs. 3-20 through 3-22, assuming $\beta = 1$. For 625 keV H ions in Si one obtains the following values (in $\text{eV}\text{\AA}^2$): $\epsilon_{v1} = 42.2$, $\epsilon_{v2} = 25.3$, and $\epsilon_v = 67.5$. In order to reproduce the random stopping value of $\epsilon_r = 108.2 \text{ eV}\text{\AA}^2$ [Zieg77a], one has to assume the core electron term to be $\epsilon_c = 40.7 \text{ eV}\text{\AA}^2$. However, the SCA calculation yields $\epsilon_c^{\text{SCA}} = 38.4 \text{ eV}\text{\AA}^2$. Therefore, in determining losses to core electrons, the impact-parameter dependence given by the L_c function is multiplied by ϵ_c corresponding to $\beta = 1$. The distributions for the $\langle 110 \rangle$ axial and the $\{111\}$ planar directions, calculated using (1) the constant density model, (2) the 2-component FEG model, and (3) the LW model, are compared with the experimental data in Fig. 3-15 ((2) and (3) are with the solid-state valence electron density). The constant density model clearly overestimates channeling energy losses, while the LW model gives too large an energy dispersion in the case of the $\langle 110 \rangle$ distribution. The 2-component FEG model is seen to reproduce features of the experimental distributions quite well for both the axial and the planar directions. These observations are consistent with a recent analysis of the H ion stopping by valence electrons in Si at lower incident energies of 50–300 keV [Lenk90].

The 2-component FEG model with the solid-state valence electron density together with the SCA model were thus used to calculate the distributions for all

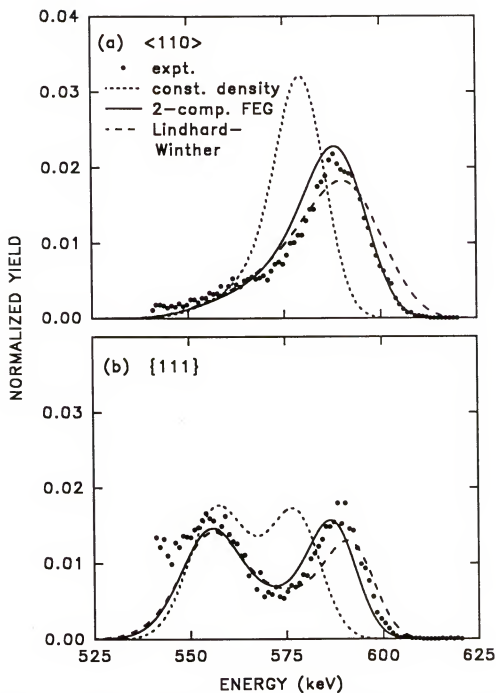


Figure 3-15. Energy distributions for (a) the $\langle 110 \rangle$ axial and (b) the $\{111\}$ planar directions, calculated using the SCA model ($\beta = 1$) and (1) the constant density, (2) the 2-component FEG, and (3) the LW models, compared with experimental data.

directions studied in the $\langle 110 \rangle$ experiment. In order to achieve the best overall agreement β was reduced to 0.94. The simulation results for a set of 12 representative distributions are compared with the experimental data in Fig. 3-16. When assessing agreement between the simulation and experiment, the low-energy part of the distributions is not taken into account, as it is affected by the overlapping Si signal (see above). The distribution for the $\langle 110 \rangle$ axial direction can still be better reproduced if $\beta = 0.97$ is used. However, the $\langle 110 \rangle$ distribution is most sensitive to crystal imperfections, and we prefer to give more weight to the distributions for other directions, in particular the $\{111\}$ planar direction at $\theta = 10^\circ$.

The present model (with $\beta = 0.94$) was also tested against our previous experiment for the $\langle 100 \rangle$ axis [Dygo94c]. The distributions simulated for 12 representative directions are compared with the experimental data in Fig. 3-17. Here, the tilt θ is referenced to the $\langle 100 \rangle$ axis, and the azimuth ϕ is taken relative to the $\{110\}$ plane. Unlike the distributions near the $\langle 110 \rangle$ axis, the distributions shown in Fig. 3-17 do not exhibit well-resolved structures. The reason for this is two-fold: first, the ratio of channeled to random energy losses for the $\langle 100 \rangle$ axis is larger than for the $\langle 110 \rangle$ axis (the channel radii for the $\langle 100 \rangle$ and $\langle 110 \rangle$ axes are $1.36 \text{ \AA}$ and $2.04 \text{ \AA}$, respectively); second, the Si crystal used in the $\langle 100 \rangle$ experiment was half the thickness of the crystal used in the $\langle 110 \rangle$ experiment, which resulted in a poorer relative energy resolution in the former case. Nevertheless, the excellent agreement between the simulated and experimental distributions shown in Fig. 3-17 gives additional support for the energy loss model used.

In the calculations above, the influence of surface layers due to C deposition during the measurements was not taken into account, as it had been found negli-

Figure 3-16. Monte Carlo simulated energy distributions (solid lines) using the SCA model together with the 2-component FEG model with the solid-state valence electron density ($\beta = 0.94$), compared with experimental data (dots) for directions near the $\langle 110 \rangle$ axis.

H beam energy 625 keV, Si crystal thickness 1.2 μm

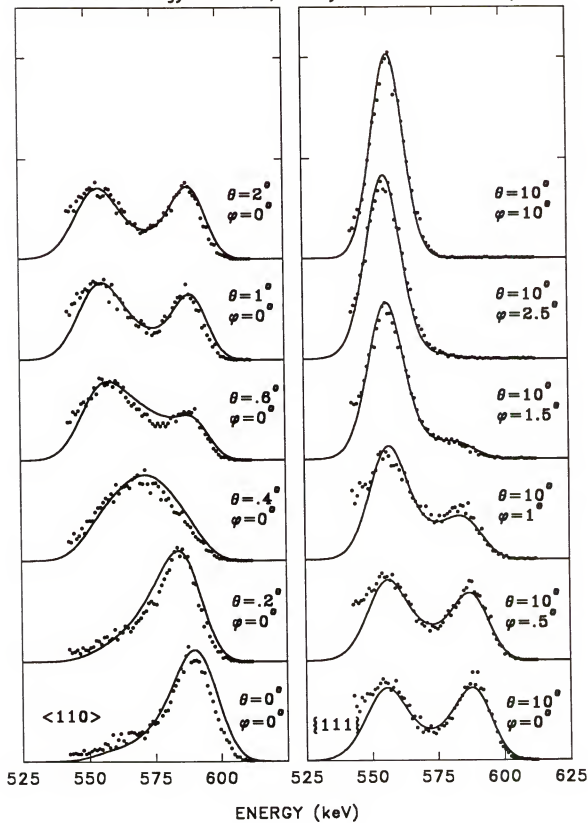
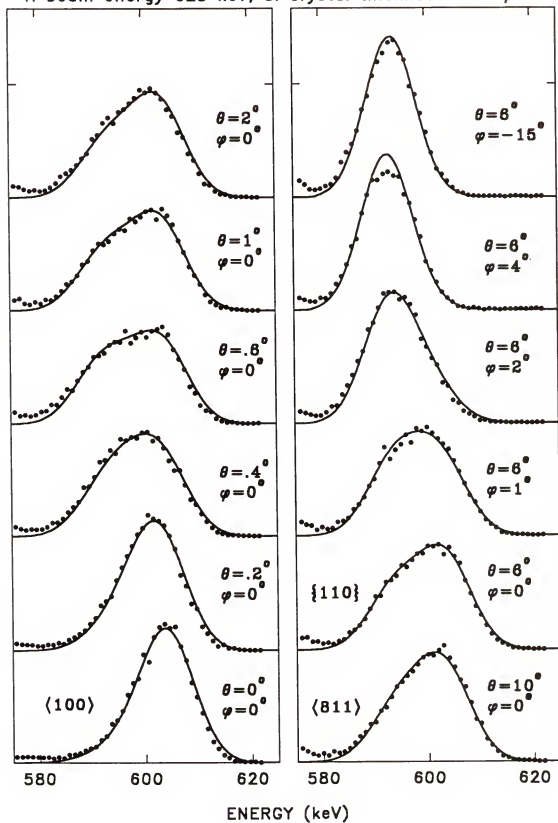


Figure 3-17. Monte Carlo simulated energy distributions (solid lines) using the SCA model together with the 2-component FEG model with the solid-state valence electron density ($\beta = 0.94$), compared with experimental data (dots) for directions near the $\langle 100 \rangle$ axis.

H beam energy 625 keV, Si crystal thickness 0.57 μm



ble in our previous study for the $\langle 100 \rangle$ direction [Dygo94c]. The distributions near the $\langle 110 \rangle$ direction, however, are more sensitive to any imperfections in the crystal. Therefore, the influence of surface layers was additionally studied in this case. The thickness of the C surface layer for the $\langle 110 \rangle$ measurement was estimated to be 5×10^{15} atoms/cm², while in the case of the $\{111\}$ planar channeling it amounts to about 3×10^{16} atoms/cm². The simulations of energy distributions were done for crystals covered with the above C layers as well as a thin silicon oxide layer (3×10^{15} O atoms/cm² and 2×10^{15} Si atoms/cm²). In comparison with the distributions obtained for perfect single crystals (without any surface layers), no significant changes in the shape of the distributions were found. One concludes, therefore, that in the case of the $\langle 110 \rangle$ experiment, the influence of surface layers on the distributions can also be neglected.

It has been shown earlier in this section that the assumption of a constant valence electron density, as compared to the non-uniform solid-state density, has a marked influence on the distributions. A related question concerns the comparison of the solid-state valence electron density versus the free-atom density. It has often been argued that the inclusion of the solid-state effects in the valence electron density is essential for a quantitative explanation of the stopping of channeled ions. The simulations have been done for the $\langle 110 \rangle$ and $\langle 100 \rangle$ axes and the $\{111\}$ and $\{110\}$ planes using the RHF valence electron density. A comparison with the simulations based on the solid-state density revealed no significant differences in the distributions, as illustrated in the case of the $\langle 110 \rangle$ axial direction in Fig. 3-18. This can be easily understood if one refers to Figs. 3-13 and 3-14 that present L_{v1} functions for the two electron densities.

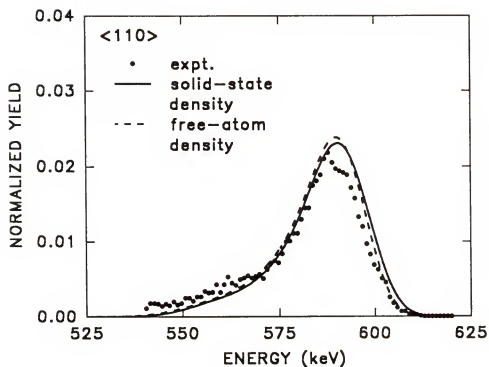


Figure 3-18. Energy distributions for the $\langle 110 \rangle$ axial direction calculated using the SCA model together with the 2-component FEG model ($\beta = 0.94$) with (1) the solid-state and (2) the free-atom valence electron densities, compared with experimental data.

The simulations were also done using the MEEA to calculate the energy loss to core electrons. The valence electron contribution to the stopping was evaluated within the 2-component FEG model with the solid-state electron density and $\beta = 0.94$. Based on the results presented earlier, the mean excitation energy of 1.4 times the binding energy was used to determine L_c . The energy distributions thus obtained show virtually no difference with respect to the calculation done using the SCA model (Fig. 3-16). This result confirms that the minor differences between the L_c functions for the two models, displayed in Fig. 3-12, are of no consequence as far as the energy distributions are concerned. In order to investigate the sensitivity of the distributions to the assumed L_c dependence, two additional simulations were done for the MEEA model with $\Omega = 1$ (see Fig. 3-12). These were for the $\langle 110 \rangle$ axis and the $\{111\}$ plane. The results are presented in Fig. 3-19, in comparison with the SCA distributions and the experimental data. The overestimation of the channeled ion energy losses by the MEEA model with $\Omega = 1$ is clearly seen.

The results presented in this section show that the experimental distributions near the $\langle 110 \rangle$ and $\langle 100 \rangle$ axes in Si can be very well reproduced by the simulation using the SCA model for core electrons and the 2-component FEG model for valence electrons. The stopping cross section for valence electrons, however, has to be reduced by 6% with respect to the values given by Eqs. 3-20 and 3-21. Also, an increase of some 10–14% with respect to the SCA prediction is needed for the energy loss to core electrons. Both the SCA and the FEG theories employed treat the ion stopping within first-order perturbation theory. Estimates of the Barkas effect within the free-electron gas model [Lind76; Sung83] give in our case about 1–2% increase of the stopping due to the Z_1^3 term in the perturbation series. Although

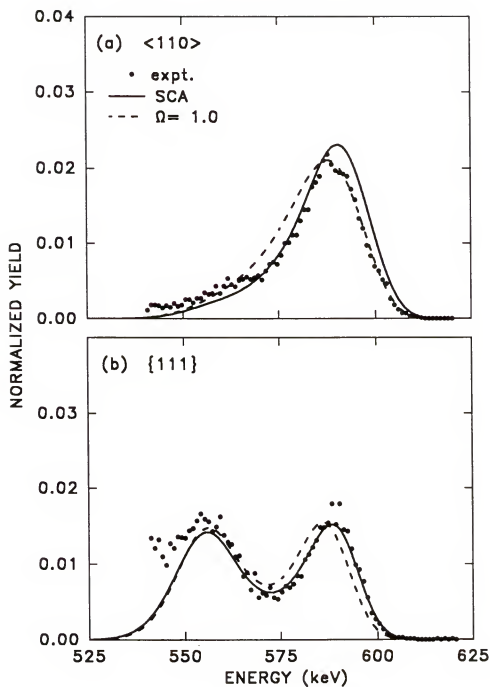


Figure 3-19. Energy distributions for (a) the $\langle 110 \rangle$ axial and (b) the $\{111\}$ planar directions, calculated using the 2-component FEG model with the solid-state valence electron density ($\beta = 0.94$) together with (1) SCA and (2) MEEA ($\Omega = 1.0$), compared with experimental data.

the Z_1^4 term is expected to be negative [Lind76; Mikk91], it does not seem likely to account for the correction of 6% found in the present work. Similarly, the negative correction for these higher-order terms in the case of the H ion stopping due to core electrons in Si, obtained in Ref. [Bala90a; Bala90b], seems to contradict the results of this study.

Analysis of Ion Trajectories. The energy distributions corresponding to the angular scan through the $\langle 110 \rangle$ axis, presented in Fig. 3-16, change rapidly with the tilt angle. A single-peak distribution for the axial direction shifts towards lower energies and broadens as the tilt increases ($\theta = 0.2^\circ$ and 0.4°). At a tilt of 0.6° , splitting of the distribution into two components is first observed. These will be referred to as the channeling and the random components. With a further increase of the tilt, the area of the channeling component increases. The observed evolution corresponds to the transition from axial to planar channeling that has been a subject of continued interest [Appl72a; Appl72b; Dell73; Smul92].

As the experimental distributions are very closely reproduced by the present simulations, it seems worthwhile to examine individual trajectories and the ion flux distribution in order to try to gain a better understanding of the observed axial-to-planar-channeling transition. Figure 3-20 shows projections of trajectories onto the interaction zone (as used in the simulation code), calculated for four tilts ($0^\circ, 0.2^\circ, 0.4^\circ$, and 0.6°). Atom rows are indicated by black dots. Each trajectory starts in the center of the $\langle 110 \rangle$ channel, and is followed to a depth of $1.2 \mu\text{m}$. If a trajectory leaves the interaction zone it is put back at an equivalent point. One can see that the trajectories for $\theta = 0^\circ$ and 0.2° are very similar. The main difference between them is that the amplitude of the transverse motion in the case

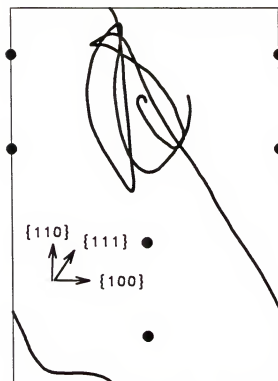
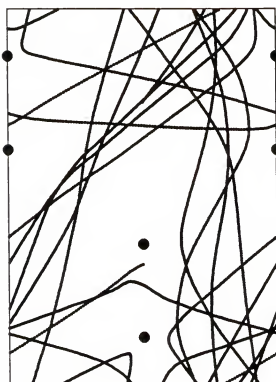
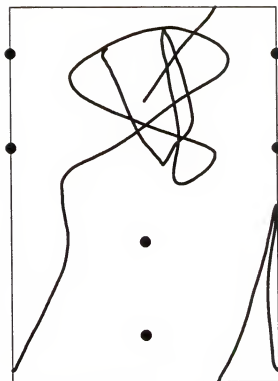
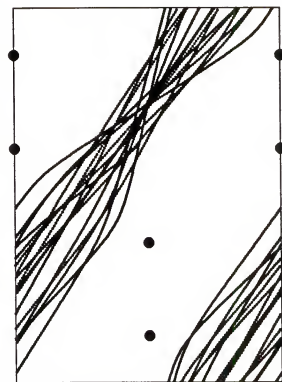
of $\theta = 0.2^\circ$ is slightly larger than that for $\theta = 0^\circ$. The trajectory for $\theta = 0.4^\circ$ penetrates almost the whole area of the channel, and it still does not display features of the $\{111\}$ planar channeling. The planar channeling is clearly seen, however, in the case of $\theta = 0.6^\circ$.

Although the above observations are based on single trajectories only, they are corroborated by the flux distributions shown for the four directions in Fig. 3-21. In each case 2000 trajectories were followed to a depth of $0.6\ \mu\text{m}$. A concentration of the flux in the central region of the channel diminishes gradually as one goes from $\theta = 0^\circ$ to $\theta = 0.2^\circ$ and on to $\theta = 0.4^\circ$. At $\theta = 0.6^\circ$, a concentration of the flux along the $\{111\}$ planar channel can be seen.

Azimuthally Averaged Mean Energy Loss Near the $\langle 110 \rangle$ Axis. In measuring the random energy loss using a single crystal one needs to avoid any channeling effects. This may prove difficult unless one knows precisely the directions that correspond to the so-called random incidence. In order to identify random-like directions, it is first necessary to know how much tilt away from the axis is needed to avoid any influence of the axis. Once a tilt has been identified as free from axial influence, a detailed study of azimuthal effects (planar channeling) must then be done to fully pinpoint random-like directions.

The first question can be best addressed by studying the energy loss for the so-called rotating axial dip, i.e. the azimuthally averaged mean energy loss as a function of the tilt angle with respect to the axis. Alternatively, one might look into the (azimuthally averaged) probability of the close encounter processes. This last approach has recently been applied for the $\langle 100 \rangle$ axis in Si [Dygo94c; Dygo94d]. We are not aware, however, of any rotating dip studies for the mean energy loss, which we

Figure 3-20. Projections of trajectories onto the interaction zone calculated for four tilts (a) 0° , (b) 0.2° , (c) 0.4° , and (d) 0.6° from the $\langle 110 \rangle$ axis. Black dots indicate atom rows.

(a) TILT = 0° (b) TILT = $.2^\circ$ (c) TILT = $.4^\circ$ (d) TILT = $.6^\circ$

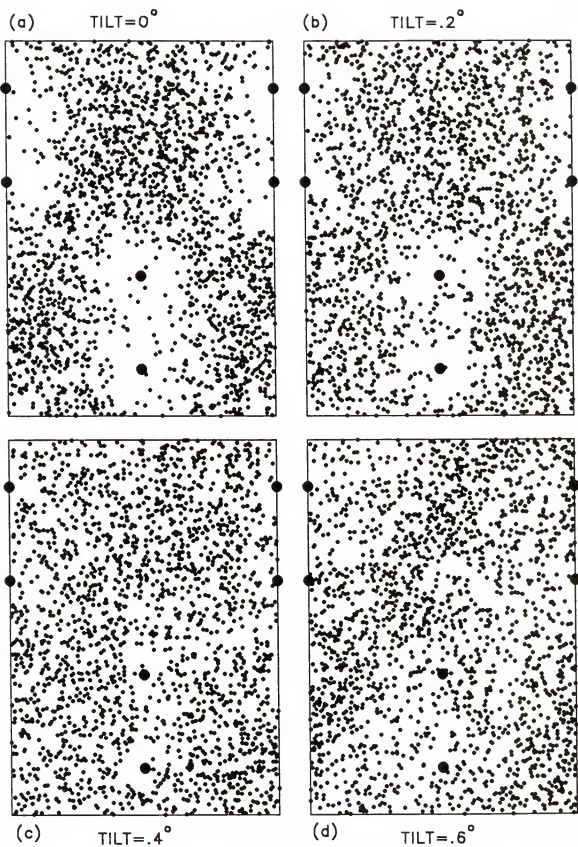


Figure 3-21. Ion flux distributions for four tilts (a) 0° , (b) 0.2° , (c) 0.4° , and (d) 0.6° from the $\langle 110 \rangle$ axis.

undertook by the simulation of the energy distributions at a number of tilts from the $\langle 110 \rangle$ axis ($0^\circ < \theta < 16^\circ$, with a step of 0.25°), using the 4-component model of Ref. [Dygo94e] (version C). At each tilt, 64000 trajectories were followed to a depth of $0.5 \mu\text{m}$. The azimuthal averaging was accomplished by randomly selecting the azimuthal angle ϕ for each incident ion within the interval $[0^\circ, 360^\circ)$, assuming uniform probability distribution. The resulting mean energy losses, normalized to the random energy loss, are presented in Fig. 3-22. The statistical uncertainty of the points shown is less than 0.2%. Although the values shown depart from the random level by a fraction of a percent only, the shoulder of the $\langle 110 \rangle$ axial dip can be seen, as well as a fine structure for tilts $\theta > 10^\circ$. One concludes that the influence of the $\langle 110 \rangle$ dip extends until tilts exceed $\theta \approx 9^\circ$. In concord with Ref. [Dygo94c; Dygo94d], the observed fine structure can be explained by the influence of planar channels tangential to the azimuthal scans at certain tilts. In the present case, the $\{123\}$, $\{158\}$, and $\{135\}$ planes were identified by means of the stereographic projection shown in Fig. 3-23.

Finally, a detailed azimuthal scan (for the mean energy loss) was calculated for the tilt of 10° used in the experiment. The results presented in Fig. 3-24 display a number of low- as well high-index planar dips. Additionally, energy losses increased by up to 5% over the random value are observed over substantial intervals of the azimuthal angle. The energy loss for the random-like direction used in the $\langle 110 \rangle$ experiment, namely, tilted by 10° off the axis, and azimuthally rotated by 10° with respect to the $\{111\}$ plane (towards the nearest $\{100\}$ plane), is seen to differ by less than 1% from the random value.

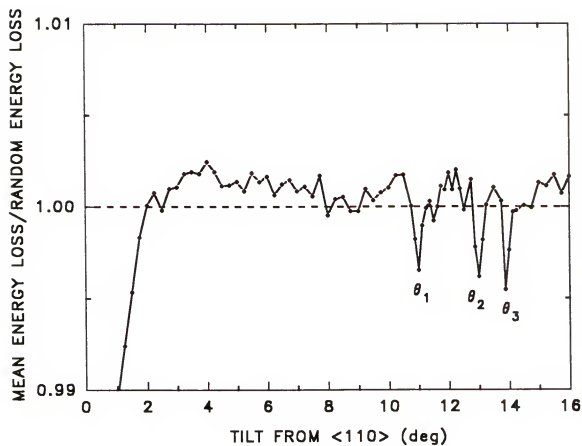


Figure 3-22. Azimuthally averaged mean energy loss (relative to the random energy loss) as a function of tilt from the $\langle 110 \rangle$ axis.

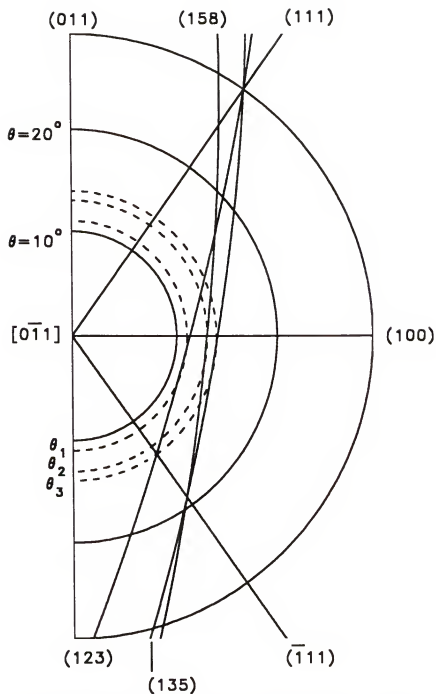


Figure 3-23. Stereographic projection for the $[0\bar{1}1]$ axis, showing various planes $((123), (158), (135))$ running tangent to the azimuthal scans for tilts θ_1 , θ_2 , and θ_3 (see Fig. 3-22).

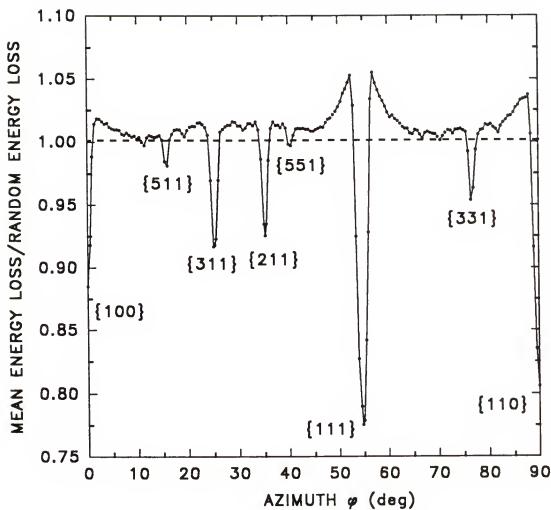


Figure 3-24. Mean energy loss (relative to the random energy loss) for an azimuthal scan taken at a tilt of 10° from the $\langle 110 \rangle$ axis.

A note concerns the identification of the high index planes in Fig. 3-23. To obtain a standard stereographic projection for the $\langle 100 \rangle$ axis, one can in principal choose Miller indices (h,k,l) of some interesting plane and obtain all the crystal coordinates corresponding to these indices. The equation

$$h \sin \theta \cos \phi + l \cos \theta = k \sin \theta \sin \phi \quad (3-23)$$

must be solved by iterating θ and solving for ϕ . The stereographic projection is obtained for the resulting ϕ solution by

$$\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} \frac{\sin \theta}{(1+\cos \theta)} \cos \phi \\ \frac{\sin \theta}{(1+\cos \theta)} \sin \phi \end{bmatrix}. \quad (3-24)$$

To obtain the projections for other axial directions, the (h,k,l) Miller indices can be transformed by the Euler angles (the rotation is from the $\langle 100 \rangle$ axis to some other arbitrary axis). The program RM.FOR [Bosh94i] produces such stereographic projections, and allows the crystal coordinates for arbitrary planes to be readily obtained.

He⁺ Near the $\langle 100 \rangle$ and $\langle 110 \rangle$ Axes

Adhering very closely to the outline presented in the previous section, in this section the energy-loss distributions for 2.5 MeV He⁺ ions (velocity unchanged from 625 keV protons) incident on silicon single crystals are studied as a function of crystal orientation (based on our paper Ref. [Bosh95b]). However, the above model is a first-order perturbation calculation for a bare nucleus, and our incident beam is He⁺. Deviations may be expected if the He⁺ ions do not become fully ionized near the surface. Incident He⁺⁺ would perhaps be better suited to our energy loss model, but He⁺ beams are readily available and thus widely used in

energy loss studies [Culb84; Jin86; Alke87; Kimu87; Naru93; Kido94] and analytical applications [Chu78].

Experiment

As the experimental procedure is nearly identical to that described in the previous section, the principal points of the procedure are given here along with any differences from the previous experiment. The incident beam of 2.5 MeV He^+ ions was produced by the UF 3.5 MV Van de Graaff accelerator. Three samples, a 0.74 μm Si(110), a 1.4 μm Si(110), and a 0.75 μm Si(100), were prepared and mounted as in the previous section. Also, the ions scattered through 65° were detected and crystal alignment was performed as discussed with the Au layer on the beam exit side, as shown in Fig. 3-25.

Each distribution was collected as before. Two angular scans were performed: (1) through the $\langle 110 \rangle$ and $\langle 100 \rangle$ axial directions along the $\{111\}$ and $\{110\}$ planar directions, and (2) perpendicular to the $\{111\}$ and $\{110\}$ planes at a tilt $\theta = 10^\circ$ and $\theta = 4^\circ$ with respect to the $\langle 110 \rangle$ and $\langle 100 \rangle$ axes for Si(110) and Si(100), respectively. The directions $(\theta, \phi) = (10^\circ, 10^\circ)$ and $(\theta, \phi) = (4^\circ, 12^\circ)$ were taken as an approximation to “random” incidence for Si(110) and Si(100), respectively [Dygo94c; Dygo94d; Dygo94f].

A number of random-like spectra were also taken to monitor and correct for carbon deposition during the irradiation, and a repeated measurement of the axial direction at the end of the experiment was used to check for structural damage due to the irradiation (found to be negligible). Finally, the sample thickness, the normalization constant for all distributions, as well as the overall energy resolution

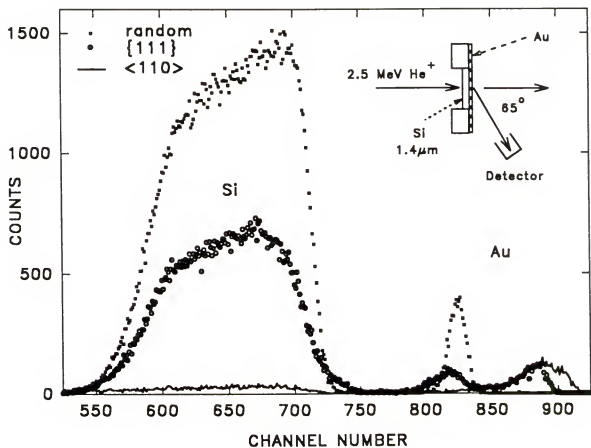


Figure 3-25. Energy spectra for 2.5 MeV He ions transmitted through 1.4 μm thick Si crystal and scattered through 65°, taken in the random, aligned with the {111} planar, and aligned with the (110) axial directions.

were determined as before. The overall energy resolution was found to be from about 15 keV to 25 keV (experiment dependent).

In order to calculate the energy loss, the simulation employs the model found to yield the best fits to the data in our study of 625 keV H^+ ions incident on silicon. Namely, the SCA model is employed for stopping due to core electrons, and the 2-component FEG model gives the stopping for valence electrons. The above model is easily adapted from 625 keV H ions to 2.5 MeV He ions by setting $Z_1^2 = 4$, as the velocity is unchanged. Based on the previous section, it was found that reducing the cross section of both components of valence stopping by 6% from the value given by the 2-component FEG theory gave the best fits to the data. Therefore, the core electron stopping cross section had to be raised by 12% from the SCA calculation so that the integral over all impact parameters reproduces the stopping cross section given in Ref. [Zieg77b]. Specifically, for 2.5 MeV He ions, $\epsilon_r = 429.5 \text{ eV } \text{\AA}^2$ [Zieg77b], $\epsilon_{v1} = 158.7 \text{ eV } \text{\AA}^2$, and $\epsilon_{v2} = 95.1 \text{ eV } \text{\AA}^2$ ($\beta = 0.94$ in both cases). Thus, $\epsilon_c^{\text{SCA}} = 175.7 \text{ eV } \text{\AA}^2$, $\sim 12\%$ larger than the SCA calculation suggests.

Results and Discussion

The simulation results for a set of 12 representative distributions are compared with the experimental data in Figs. 3-26, 3-27, and 3-28. Figure 3-26 is for a $0.74 \mu\text{m}$ Si(110) sample, Fig. 3-27 is for a $1.4 \mu\text{m}$ Si(110) sample, and Fig. 3-28 is for a $0.75 \mu\text{m}$ Si(100) sample. It is evident from the comparisons that the data can be reasonably well reproduced using the energy loss model discussed. It is also clear from the data that systematic deviations between experiment and theory exist that were not present in the H^+ incident ion case [Dygo94f]. The deviations between

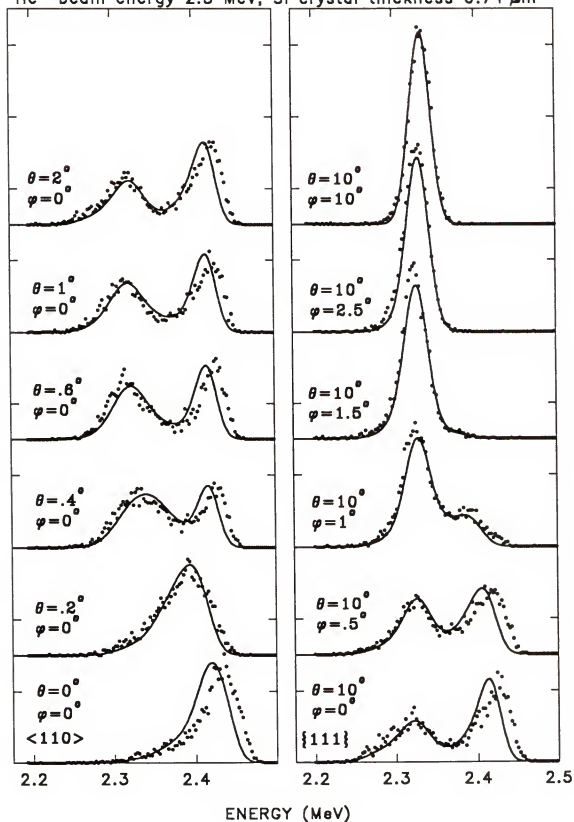
theory and experiment in all data sets are pronounced on the high energy side of the energy distributions, where the simulated distributions are shifted to lower energies with respect to the data. Further, scans near the $\langle 100 \rangle$ axis (Fig. 3-28) match the theory better than either scan near the $\langle 110 \rangle$ axis (Figs. 3-26 and 3-27), and scans performed on the $1.4 \mu\text{m}$ Si(110) sample are predicted by the theory better than scans on the thinner $0.74 \mu\text{m}$ Si(110) sample. Finally, one notices that the point $(\theta, \phi) = (0.2, 0)$ is reproduced by the theory surprisingly well in Figs. 3-26 and 3-27, even though it is surrounded by points exhibiting marked deviations. We will try to address these issues.

The first point that must be made concerns the fact that the incident beam in the experiments was He^+ rather than He^{++} , while the energy loss model employed assumes a bare nucleus (He^{++} ion) within the silicon crystal. In random incidence or amorphous targets, one may assume that after some “short” ($5 \text{ \AA}$ in silicon [Arms65]) distance within the crystal, virtually all 2.5 MeV He^+ ions (more than 95%) are stripped and become He^{++} ions, making the energy loss model fully applicable. The channeling effect, however, steers many ions “far” ($1 - 2 \text{ \AA}$) away from the host atoms, keeping them in a reduced electron density, and the tendency to lose a second electron is reduced. Therefore, an important difference from the H^+ ion experiment is introduced: well-channeled partially stripped He^+ ions may survive to large penetration depths.

The disagreement between theory and experiment can be explained in terms of the above supposition in that well-channeled He^+ ions would suffer substantially reduced stopping compared to the assumed model [Loga92]. This would shift the high energy side of the simulated distributions to lower energy as compared to the data,

Figure 3-26. Monte Carlo simulated energy distributions (solid lines) using the energy loss model described in the text compared with experimental data (dots) for directions near the $\langle 110 \rangle$ axis (Si crystal thickness $0.74 \mu\text{m}$).

He⁺ beam energy 2.5 MeV, Si crystal thickness 0.74 μm



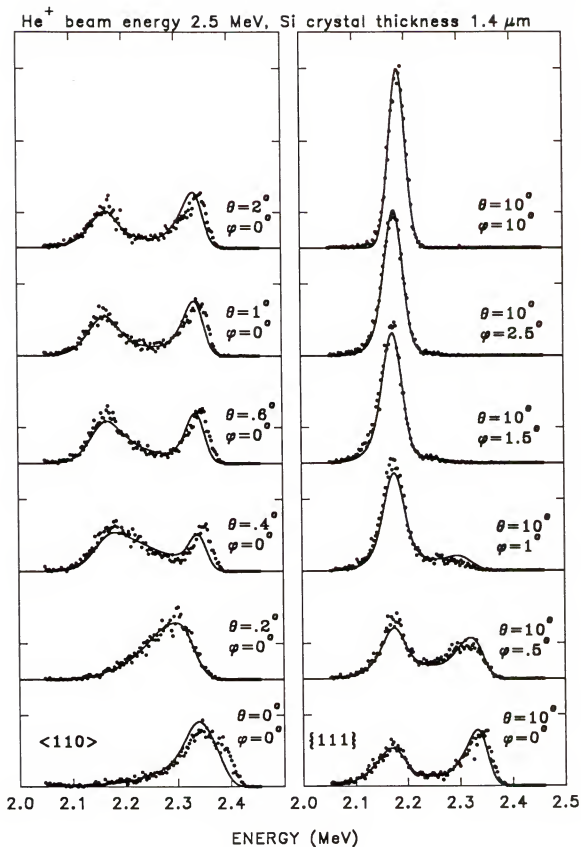


Figure 3-27. Same as Fig. 2 but for 1.4 μm thick Si.

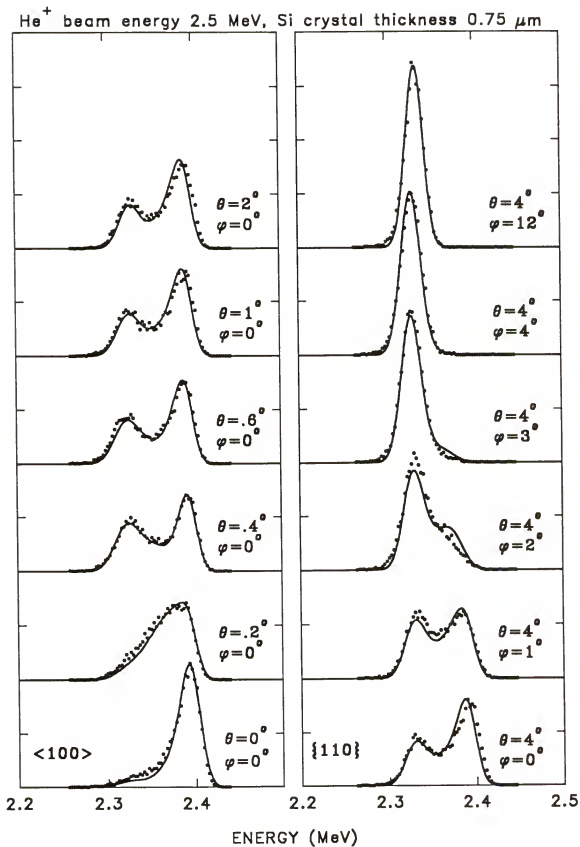


Figure 3-28. Same as Fig. 2 but for directions near the $\langle 100 \rangle$ axis and 0.75 μm thick Si.

since the high energy side corresponds to well-channeled particles and the simulation assumes the enhanced stopping of a bare nucleus for all ions. The low energy side of the simulated distributions would be expected to agree with the measured distributions since ions moving close to atomic strings will be completely ionized much more quickly. In this way, the overall deviation between experiment and theory can be qualitatively explained by the He^+ incident beam. This explanation seems to be at variance with the conclusions concerning the survival rate of 2 MeV He^+ ions in GaAs:Er, found in Ref. [Kido94] (no difference in stopping between singly and doubly charged helium ions was found).

In considering the differences in the deviation between the data sets, since the $\langle 100 \rangle$ channel has a smaller radius than the $\langle 110 \rangle$ channel (1.36 Å compared to 2.04 Å) and a larger electron density in the middle of the channel as a result [Dygo94f], one might expect even well-channeled He^+ incident ions to be fully stripped near the surface. This would explain the better agreement between theory and experiment in the $\langle 100 \rangle$ experiment than either $\langle 110 \rangle$ experiment. In addition, the 1.4 μm Si(110) scans agree better with the theory than the 0.74 μm Si(110) scans, and this may be due to the fact that the ions spend more time completely stripped penetrating the thicker crystal. The absolute (dis)agreement with experiment should be roughly the same then, but the relative (dis)agreement is much improved in the thicker sample's scans as the partially stripped ions survive for some penetration depth which is a smaller fraction of the total distance travelled in the thicker sample (shift between simulation and experiment for the axial direction is 16 keV for Fig. 3-26 and 19 keV for Fig. 3-27).

A final point concerns the apparent anomalous agreement between the simulation and experiment for the point $(\theta, \phi) = (0.2, 0)$ in Figs. 3-26 and 3-27 even though surrounding data points display deviations. This can be explained in terms of the axial to planar channeling transition. As shown in the previous section, there is a region in the axial to planar channeling transition where axial channeling is suppressed due to the tilt from the axis, but planar channeling has not yet manifested itself. Therefore, there is simply no sizeable well-channeled component of the beam at this point, and the He^+ ions become fully stripped near the surface.

CHAPTER 4

DATA ACQUISITION AND REDUCTION

Now we will switch gears somewhat. Chapter 3 dealt with experiments performed in the RBS scattering chamber. The rest of this dissertation will deal with experiments performed in the UHV scattering chamber as we will be concerned specifically with physics at surfaces, and require UHV conditions to maintain clean surfaces. We will, however, be relying heavily on results from Chapter 3, but the method of data acquisition, reduction, and analysis will be significantly different.

Beam to Sample Alignment

The method of beam-sample alignment for the UHV scattering chamber is of necessity different as stepper motors are not available. However, a piece of quartz at the end of the beam-line is more than sufficient for locating planes and axes, as the quartz fluoresces, clearly showing a blocking pattern [Feld82]. That is, high symmetry directions are blocked due to the regular arrangement of the silicon atoms, and show up as dark areas. When aligned directly with a high symmetry direction, though, the beam appears as a bright spot due to the channeling effect, as the beam is now steered along the low index directions by the atom rows.

We are also interested in aligning the crystal as fast as possible to minimize the degradation of our surfaces (even at UHV, eventually the surfaces will get contaminated). We have arrived at a method which allows crystal alignment to be achieved in ~ 5 min, but the accuracy is somewhat limited as the directions are

found by eye $\sim \pm 0.05^\circ$. Typically our data are acquired for directions near the $\langle 100 \rangle$ axis first as these data yield the most useful information [Bosh95c]. The procedure is to roughly find the $\langle 100 \rangle$ direction at a point on the sample where data will not be taken. Then one moves to the desired area of the sample for data acquisition, and the reference plane is carefully found and noted (usually chosen to be the $\{100\}$ plane). Now the $\langle 100 \rangle$ is carefully found, and an energy spectrum is immediately acquired as axial directions are the most sensitive to irradiation damage. While this spectrum is acquired, the reference directions are input into an orientation program, ORIENT.FOR [Bosh94f], which uses the methodology outlined in Chapter 3 [Dygo93c] to convert between lab and crystal coordinates ((θ, ϕ) represent tilt and azimuth respectively in crystal coordinates, and similarly, (A,C) for laboratory coordinates). It accepts as input all the crystal coordinates of interest, and outputs the goniometer positions for these directions. All the desired data are now acquired by moving the goniometer to the specified coordinates. For directions close to the $\langle 110 \rangle$ axis, the procedure is the same except a reference plane need not be found as the $\langle 100 \rangle$ axis can serve this purpose (the two axes are joined by a $\{100\}$ plane).

There are some notable special requirements of the UHV scattering chamber. First, γ (the angle between the sample surface plane and true verticality) can not be found in any reliable way as the goniometer arm is moved each time a sample is transferred [Seib93], but it is estimated to be $< 1^\circ$ by monitoring a horizontal plane to large tilt angles as discussed in Chapter 3 [Dygo93c]. However, the principle reason for an entirely new crystal orientation program is that angle A is obtained to an accuracy of 0.02° from a dial in which one revolution is 3.6° . This creates

mathematical complications which are dealt with in ORIENT.FOR; dial and exact tilt angle are not related in a straightforward way. Table 4-1 shows output from ORIENT.FOR.

Table 4-1. Sample output from ORIENT.FOR.

Direction	ref axis/plane	Crystal coord's		angle A	Lab coord's	
		θ	ϕ		dial reading	angle C
$\langle 100 \rangle$	$\langle 100 \rangle / \{100\}$	0.00	11.00	307.58	129.	170.78
$\{110\}$		6.00	45.00	313.60	70.	166.12
rnd		6.00	30.00	313.52	66.	175.45
$\langle 110 \rangle$	$\langle 110 \rangle / \langle 100 \rangle$	0.00	10.00	350.94	137.	123.02
$\{111\}$		8.00	54.74	347.13	127.	133.03
rnd		8.00	64.74	348.44	12.	133.68

It was eventually found that angle C gave irreproducible rotations, possibly due to slipping in the vernier dial used to change the angle. Therefore, a modified procedure (applicable to Chapter 6) was developed to minimize (essentially eliminate) errors introduced in this way. However, the traditional angular scan was abandoned as a result, though overall adsorbate yield still played an important role. Basically, we restricted our data acquisition to directions that are found well by eye (axial directions, $\pm 0.02^\circ$) and directions where small inaccuracies are not important, determined by simulations (planar directions tilted by $6^\circ - 8^\circ$ from axes and random directions). In practice, one finds and takes data in the axial direction, finds and takes data in one or more well-defined planar directions, and then uses ORIENT.FOR and the reference directions just located to find random directions (random directions that approximate amorphous targets were found in Chapter 3).

Transmission Energy Axis Calibration

Our energy spectra are typically acquired in a transmission geometry with fixed detectors located at $< 90^\circ$, specifically, 70° and 79° (see Fig. 4-1) [Seib93]. This makes the process of calibrating the energy axis of these detectors somewhat more complicated than that previously discussed as the silicon thin window must be penetrated by the ion beam before scattering into these detectors. Thus, the energy lost by the beam during silicon window penetration must be taken into account so that the energy of the beam at the beam-exit surface is known. If the beam energy at the beam-exit surface is known, then the kinematic factors (for the appropriate scattering angles) for scattering from silicon and whatever adsorbates are present can be utilized to calibrate the energy axis.

The problem that arises is that in order to account for the energy lost by the beam while traversing the sample, the silicon thickness must be known. In order to find this thickness, we require the use of the 150° detector (see Fig. 4-1) which can be readily energy calibrated in advance by turning the sample so that the adsorbates are facing the detector and using the method described in Chapter 2. Further, since we are dealing with single crystal silicon windows, we must be careful to align the beam away from major crystallographic directions ("random" beam-sample orientation) so that the energy loss tables valid for helium penetrating amorphous silicon are in effect. Locating such directions has been discussed in Chapter 3.

Once we are aligned with such a direction, we can find the silicon thickness using techniques previously discussed with the 150° detector. As the detectors all collect data simultaneously, the thickness found from the 150° detector is identical

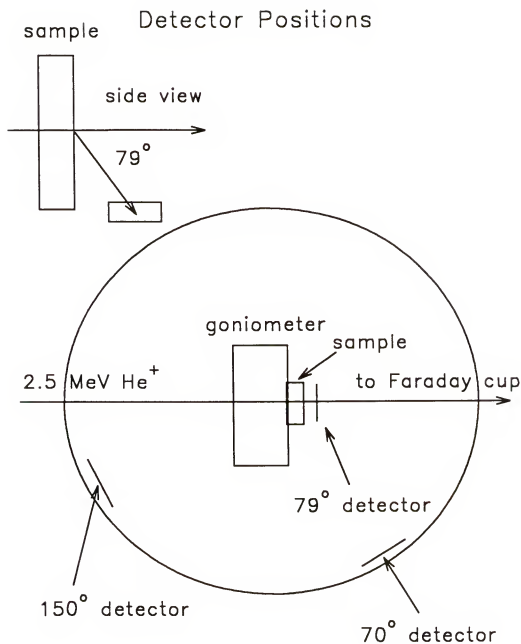


Figure 4-1. View from the top of the scattering chamber showing the various detector positions. The detector at 150° (same height as sample) can be readily calibrated and then the silicon thickness found. The detectors at 70° (also sample height) and 79° (located below the sample, see inset) can be energy calibrated using the determined silicon thickness.

in all detectors. Now we can use HESTOP.FOR to find the energy of the beam after penetrating the silicon window (taking any geometrical considerations into account), and use the kinematic factors of the various materials to calibrate the energy axes of the transmission detectors, using ECALIB.FOR.

Figure 4-2 shows a typical energy spectrum obtained from a transmission detector for $\langle 100 \rangle$ aligned and random beam-sample orientations. Both Sb and Ge have been deposited on the beam-exit surface. Again, for now, we consider just the random orientation as the energy loss of helium ions in amorphous silicon is well-known [Zieg77b]. The high energy side of the silicon peak (point labeled 1; the half-height is taken to account for detector resolution) corresponds to scattering as the beam is exiting the crystal. If the beam scatters earlier, it will greatly increase its path length through the silicon (for the geometry shown in the inset), reducing the energy registered by the detector. Note that Sb is present on both surfaces of the silicon (the high energy peak again corresponds to scattering at the beam-exit surface), and allows the 150° detector to be energy calibrated without turning the sample around. Having the energy at the beam-exit surface using the procedure outlined above, we can use points 1, 2, and 3 to obtain an accurate energy calibration.

A problem can arise, however, when beam-sample orientation is changed. Typically, we have small thickness variations ($\sim 10\%$) when the beam spot on the sample is altered by moving the goniometer. However, armed with the energy calibration, we can obtain the silicon thickness by reading off the high energy edge silicon channel number, converting to an energy, and using HESTOP.FOR to obtain the thickness. This works because the silicon signal is obtained almost exclusively from

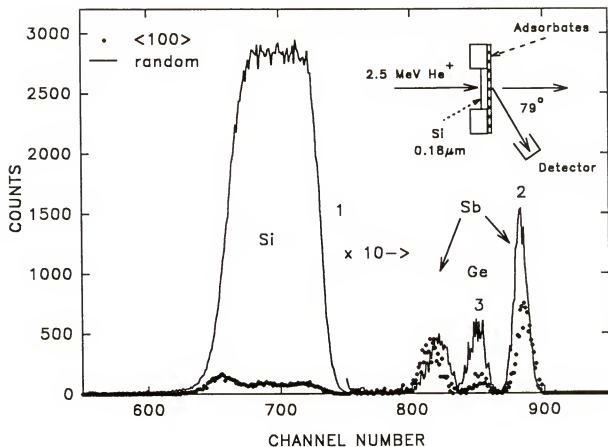


Figure 4-2. Sample energy spectra in the transmission geometry for $\langle 100 \rangle$ aligned and random beam-sample orientations. The high energy peaks correspond to scattering from the beam-exit side of the thin window (see inset) as scattering when the beam enters the target will result in a much longer path length through the sample to the detector. Knowing the Si thickness in a random orientation (from the 150° detector), the energy of the beam at the beam-exit surface can be found from energy loss considerations. Then, the kinematic factors of Si, Sb, and Ge (points labeled 1, 2, and 3) can be used to generate an accurate energy calibration.

non-channeled helium ions [Feld82], so they experience the energy loss corresponding to an amorphous target. This is not true of the Sb and Ge signals, which are greatly affected by the beam-sample orientation, so we must already have the energy calibration from a random orientation [Bosh96]. The above procedure is necessary for directions close to the $\langle 110 \rangle$ axis where beam spot can change drastically with crystal orientation as the sample is tilted by 45° .

Experimental Energy Distributions

The data must now be put into a form usable to the simulation program that will be discussed in the next chapter. Usually, the 79° energy spectra are favored because of the greater mass separation obtained in this detector (due to the kinematic factor at 79°). However, occasionally this detector can be partially blocked by goniometer parts (due to the near 90° scattering angle) in which case the yields are taken from the 70° detector. This latter detector can itself have problems due to the compression of the acquired energy spectra (kinematic factors for all atoms are approaching unity with smaller scattering angle) and this makes the yield calculation for the interesting peaks difficult, as their separation from the Si and Sb from the other side is not sufficient. Thus, it becomes advantageous to separate the energy distributions and yield calculations in analyzing the data, as there is some uncertainty in the yield calculations. We therefore normalize the energy distributions to a given total peak area. In this way, the 79° detector can still be used for energy spectra despite possible blocking effects, as the spectra will be normalized. Each spectrum is acquired for $24 \mu\text{C}$ of the integrated beam charge to allow adequate statistics in the energy distributions for submonolayer adsorbate coverages.

One must first decide upon the region of the energy spectrum that is of interest. Of course, this includes all peaks of interest, but also a reasonable region surrounding the peaks is chosen if a fit to the background is desired. The counts (the yield) in the selected region are summed and recorded (as yield versus tilt from the axis) in a file as this information will be lost when the data are normalized for simulation purposes. The scattering yield is normalized so that the yield for "random" incidence is one.

The channel number in the selected region is converted using the energy calibration for the appropriate detector. The counts at each channel are then divided by the yield (total counts in the region). The counts are further scaled by (energy calibration slope/2) as the simulation program creates simulated energy spectra with a 2 keV bin width (see Chapter 5). Thus, both the data and the simulation will have the same integrated area of two. The data reduction is accomplished by the program STEDN.FOR [Bosh94e], and Fig. 4-3 shows a sample spectra before and after the reduction. An uninteresting peak is not selected (Sb on the beam-entrance surface) and the large yield differences evident in the raw data are lost after normalization, but the yield is noted as this will be important information that will complement the energy spectra.

Recently, a modification to this normalization scheme has been made. If the yield for the interesting region in the 70° detector can be accurately obtained, then an improved scheme is to combine the yield and energy distribution information together by adjusting the simulated energy distributions by the ratio of simulated to experimental yields (relative to the respective random yields) obtained from the 70° detector before comparison with the (79°) experimental distributions (see Chapter

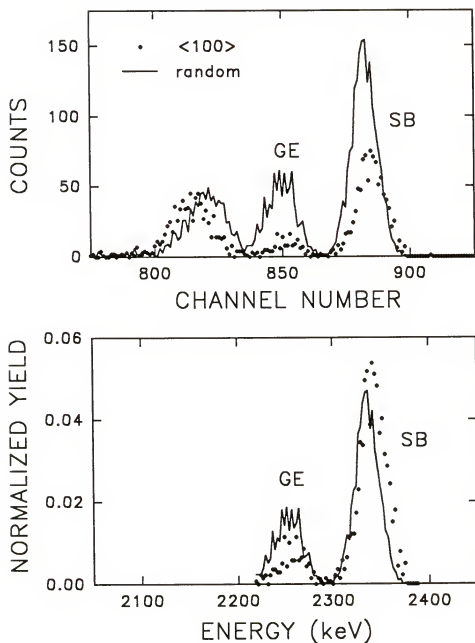


Figure 4-3. Comparison of data before and after reduction for $\langle 100 \rangle$ aligned (dots) and random orientations (solid line). First, channel number is converted to energy using the energy calibration for a transmission detector. Then, the region of interest (Ge and Sb peaks at beam-exit surface) is summed and the data normalized so that the integrated area in the region of interest is two.

6). An even better improvement would be to fix the periodic blocking problem for the 79° , normalizing the simulated energy distributions to this relative yield. The latter improvement is currently being addressed.

Linear Background Fit

A final reduction point concerns the fitting of background (noise) counts. The background will not be subtracted from the data, rather the simulated spectra will be modified based on the fit parameters to simulate the background, basically adding in counts to the simulated spectra.

The background can be well-approximated by a linear fit. The fit is accomplished by the Levenberg-Marquardt Method. The FORTRAN code was obtained from Numerical Recipes in FORTRAN [Pres92], and modified (LINE.FOR [Bosh95a]) to generate linear fits to supplied data.

The region of interest of the energy spectrum is read in by the program. It is different for each crystal orientation because of the energy loss of channeled ions (see Chapter 3). This region includes a reasonable area surrounding the spectrum peaks (at least as many channels as the peaks themselves occupy). Since we are fitting the background, the number of background channels need not be the same as the signal, but it is desirable to have the included backgrounds on either side of the signal the same size. Table 4-2 shows some details of the fitting procedure. The signal and background regions are in channel numbers, but are converted in the fitting program to energies using the energy calibration. Interference from the silicon signal or other uninteresting peaks may make it necessary to weight the background on one side of the peaks, usually the high energy side, causing an underestimation of the background, as the background is smaller at high energies.

Further, the peak region itself is specified, and this region is then excluded from the fit. Thus, the actual fit is only performed on the background counts to the right and to the left of the spectrum peaks. Figure 4-4 shows a sample spectrum (dots) and the accompanying linear background fit. The fit is especially good in the region where the peaks are actually located.

Table 4-2. Background fit using LINE.FOR. The signal and background regions are in channels. The slope is $\times 10^{-6} \frac{\text{normalized counts}}{\text{keV}}$, and the intercept is $\times 10^{-3}$ normalized counts.

Signal	Left Background	Right Background	Slope	Intercept
776-864	712-775	865-929	-1.2	2.9
777-871	723-776	872-926	-1.0	2.5
790-854	743-789	855-902	-2.1	5.0
775-871	710-774	872-937	-1.2	2.9
779-869	724-778	870-925	-1.3	3.2
796-858	743-795	859-912	-1.7	4.2

In order to subtract background from yield calculations, where fitting parameters are not needed, a similar linear background fit is performed by the program BK.FOR [Bosh94g]. This program takes the supplied peak region and sums the counts. It then calculates an equal size region on the right and left of the peak region and sums this background. The net yield is then found by subtracting the background counts from the total yield in the peak region. This program can also weight background to one side of the peak region if interference of some sort is present in the energy spectrum. However, the overall background must be the same number of channels as the signal.

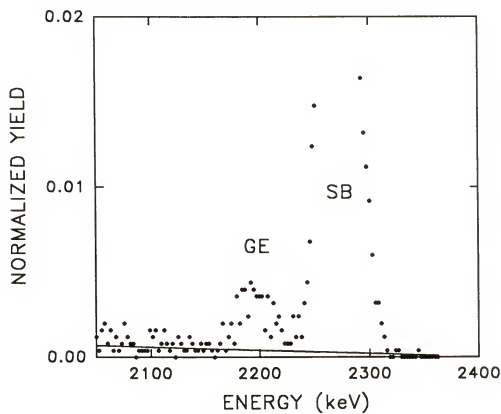


Figure 4-4. Data (dots) with background noise and a linear fit to the noise. The noise is not subtracted from the data, but the fit parameters are used in simulating the data.

CHAPTER 5 SITE DETERMINATION USING ENERGY DISTRIBUTIONS

Simulation of Adsorbate Energy Distributions

Obtaining Monte Carlo Output

The first task is to obtain ion positions and energies within a basic channel. This is readily accomplished using a modification of the channeling simulation programs described in Chapter 3. The program is exactly the same with the minor exception that ion positions and energies when they have completed their journey through the crystal are outputted to a file. The file can be either ascii (C18ASC.FOR) or binary (C18BIN.FOR) format, with binary being the preferred choice due to the substantially smaller file size (only 25% of the ascii output). The disadvantage is that the binary format takes longer to read into the site determination program that will be discussed.

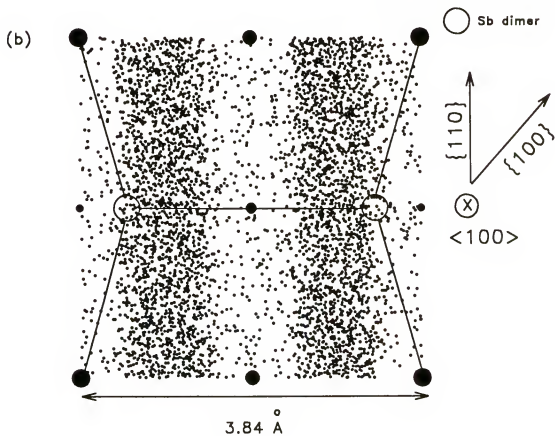
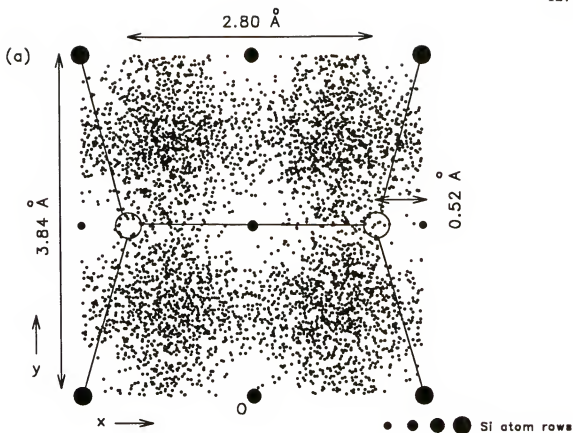
Typically, 20,000 ions are followed for a given crystallographic direction and silicon thickness (the silicon thickness can vary somewhat for different crystal orientations due to new beam spots, but this is readily accounted for, see Chapter 4). The large number of ions ensures that adequate statistics will be achieved throughout the channel, even in regions where not many ions are expected due to the channeling effect (near atom rows) [Feld82]. This results in a binary file size of about 0.25 megabytes (MB). Thus, the ascii output is simply too large if many crystal coordinates are investigated, and a typical angular scan near a single axial direction involves roughly ten such points.

The program SITE.FOR [Bosh94c] now reads in the positions and energies of all of the ions in a specified Monte Carlo output file. As the Monte Carlo program can simulate ion trajectories for directions close to both the $\langle 100 \rangle$ and $\langle 110 \rangle$ axes, SITE.FOR was written to also handle directions close to these two axes. A few changes must be made to the ion positions due to different coordinate systems between the programs. Further, the coordinate systems used between axes are different as the geometry of Si atoms seen by the beam is quite different for the two axes (see Figs. 5-1 through 5-3). In particular, the ion coordinates for directions near the $\langle 100 \rangle$ axis are scaled and moved into a single channel (the basic channel), as the Monte Carlo output actually covers four channels (the interaction zone from Chapter 3), as shown in Fig. 5-1. This can be done due to the symmetry of the problem, and greatly improves the statistics (high areal density of ion positions). For directions near the $\langle 110 \rangle$ axis, the ion coordinates are scaled and shifted as the basic channels investigated by the Monte Carlo and site programs have different origins. There is no extra gain in statistics in this case as the Monte Carlo program itself considers just one channel (again, the interaction zone of Chapter 3), shown in Fig. 5-3. The statistics are poorer still for these directions as the basic $\langle 110 \rangle$ channel is so much larger than the $\langle 100 \rangle$ axis.

Obtaining Trial Site Coordinates

Now we have all the ion positions and energies in coordinates useful to the site program (SITE.FOR). Next we need to input the trial adsorbate position. The input is given in coordinates on the Si(100) surface with the origin placed above the silicon atom row nearest the surface. The coordinates are in fractions of a lattice constant (for Si, the lattice constant is 5.431 Å). The silicon atoms closest to the surface

Figure 5-1. View of the Si(100) surface from above. Large black dots are Si atom rows and small dots are ion positions a) when exiting the Si crystal aligned with the $\langle 100 \rangle$ axis, and b) when exiting aligned with the $\{110\}$ plane (at a tilt of 6° from the $\langle 100 \rangle$ axis). The open circles are Sb positions in the Si surface plane. Sb positions are overlapped with the ion flux distribution to obtain a simulated scattering yield and energy distribution for that site which is compared with experimental data.



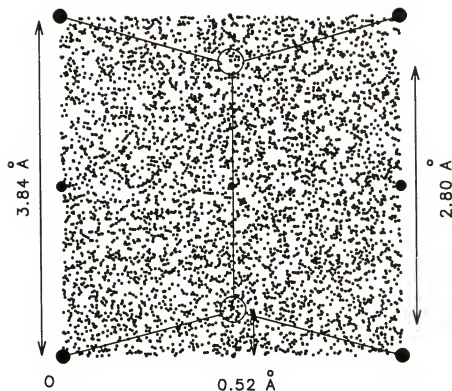
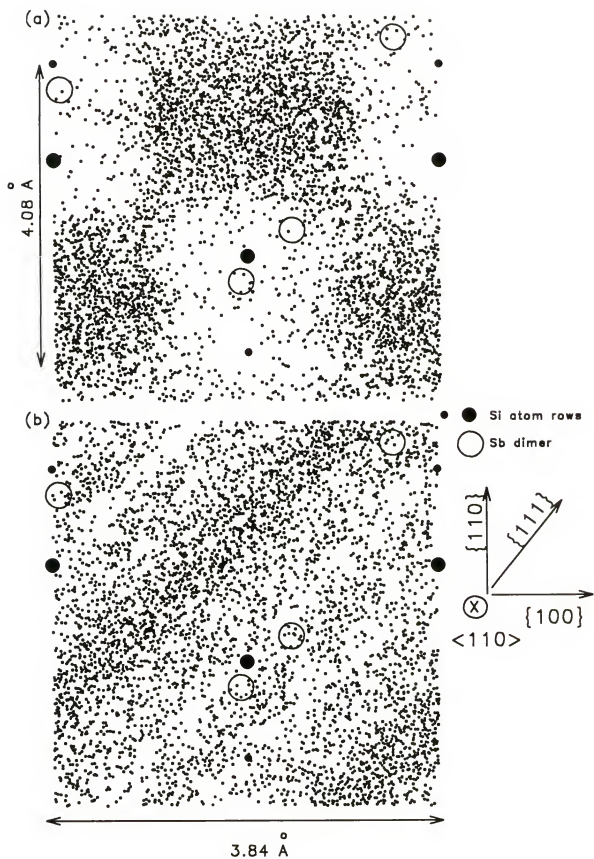


Figure 5-2. Same as Fig. 5-1 except that the Si(100) atomic arrangement corresponds to a single down step from Fig. 5-1. This results in a rotated Sb dimer on the surface which must be accounted for in the site program. Further, the ion positions those are after exiting the crystal aligned with a "random" direction. Note the even distribution of ion positions over the channel; there is no evident channeling effect for this orientation.

Figure 5-3. View of the Sb dimers when the crystal is aligned near the $\langle 110 \rangle$ axis. Again, large black dots are silicon atoms rows and small dots are ion positions when exiting the crystal a) aligned with the $\langle 110 \rangle$ axis, and b) aligned with the $\{111\}$ plane (at a tilt of 8° from the $\langle 110 \rangle$ axis). The four Sb positions (open circles) correspond to the Sb positions from the previous figures (inputted $\langle 100 \rangle$ positions) transformed to the coordinate system relative to the new axial direction. Each Sb dimer member yields a different position when aligned in this direction, and there are two more for the rotated dimer from a step.



defining the basic channel have the following coordinates: $(x, y, z) = (.354, 0, -.25)$, $(0, 0, -.50)$, $(0, .354, -.75)$, $(.354, .354, -1.00)$ (the origin in Fig. 5-1 is marked O). The basic channel is $1.92 \text{ \AA}$ square, so $1.92/5.43=0.354$, thus the x and y coordinates. Also, the distance between atomic planes for this axis is $1.36 \text{ \AA}$, and $1.36/5.43=0.25$, thus the z coordinate. Note that z is chosen to be positive above the crystal so that the adsorbate will have $z = 0$ if it continued the silicon lattice structure in that direction. To illustrate, if one wanted to investigate a perfectly substitutional adsorbate position, one would input the coordinates $(.354, .354, 0)$.

To test the site program, we used a well-studied system, Sb on Si(100) (see next section), so that will be our standing example for now. In order to tie up the one remaining Sb bond on each atom (each Sb atom has three bonds, and two are employed bonding to the substrate), the two Sb atoms “dimerize”, moving toward each other, and bonding. Since this movement is identical for both Sb atoms, they are said to form symmetric dimers (a modified bridge site) on the Si(100) surface (see Ref. [Gran94a] for a detailed discussion of the Si(100) surface). Referring to Fig. 5-1 and 5-2, we can see what the actual Si(100) surface looks like, complete with Sb dimers. Further, we can clearly see axial and planar channeling evident in the ion flux distribution (small dots). Figure 5-2 shows no such channeling effect; the ion distribution is uniform over the channel for “random” incidence.

Using the coordinate system described above, the Sb positions for Fig. 5-1 are $(.258, .354, 0)$ and $(-.258, .354, 0)$. Further, the surface has regular steps (illustrated in Fig. 5-2 as a step down), rotating the Sb dimers. These rotated dimers have coordinates $(.354, .096, -.25)$ and $(.354, .612, -.25)$. However, the z coordinate can be reset to zero since we have a new surface plane. The terrace area of the two types

of steps is assumed to be of equal size, so all of the Sb positions must be considered equally (the beam spot covers many steps of both varieties). However, the program has recently been modified to allow unequal step size densities (see Chapter 6).

The site program considers just one basic channel, and most of the Sb positions in Figs. 5-1 and 5-2 are not in the basic channel. Due to the symmetry of the problem, the sites can all easily be put into the basic channel. For the coordinates given above, and considering directions near the $\langle 100 \rangle$ axis, this means eliminating the negative x sign for the second member of the non-rotated Sb dimer, putting this member in the basic channel by a reflection about the y-axis. The symmetry of the problem further allows us to include the rotated pair in the calculation by simply interchanging the x and y coordinates of the non-rotated pair. Thus, one need only input the sites for the non-rotated dimer pair, as the rotated pair is automatically included (this rotated pair is referred to as an equivalent site). For our particular example of Sb on Si(100), two sites are repeated after moving the sites into the basic channel, since we have symmetric dimers. We then need input only one site. However, the more general case of asymmetric dimers (displacement toward each other is not the same for the two atoms) can readily be handled by the program, as the site program allows two independent sites to be inputted.

A problem still exists if part of an adsorbate site partially leaves the basic channel (if it resides on the edge of the basic channel, for example). We must correct for the part of the site that is not properly overlapping ion positions. This is done by artificially inserting extra sites, and is illustrated in Fig. 5-4 still using our example of Sb on Si(100). The site labeled 1 is the inputted site, (.258,.354,0), and site 2 represents the contribution from the rotated dimer, (.354,.258,0). Sites 3

and 4 are the artificial sites that account for the parts of sites 1 and 2 that will not overlap ions (since they are on the border between channels). In fact, they properly simulate an overflow into another channel by being shifted across the channel. Site 5, a perfectly interstitial site, has the same position (relative to the basic channel) whether rotated or not, and since it doesn't reside near the channel edge, needs no corrective sites.

Let us briefly consider the $\langle 110 \rangle$ axis. Referring to Fig. 5-3, we can see several Sb positions now. This is because there are more equivalent sites for this direction and they must all be taken into account. Each member of a dimer pair gives a different site, and we must consider both rotated and non-rotated dimers. Further, an asymmetric dimer has two possible orientations, and this gives us twice as many equivalent sites, for a total of eight. Indeed, the equivalent sites can be found quite easily using the Euler angles (Eq. 5-1) and the proper rotations (Table 5-1) along with the inputted positions for the $\langle 100 \rangle$ axis [Gran94a]. In practice, the transformations are already hard-coded into the program. The inputted coordinates for the $\langle 100 \rangle$ are simply used to evaluate the transformation expressions. As before, once the transformed sites are found, the sites must be shifted into the basic channel. In addition, corrective sites are again necessary. It should be noted that since this channel is so large, ions near the center do not lose energy in the way described in Chapter 3, since the penetrating helium ions are not fully stripped near the surface [Bosh95b]. However, since the Sb positions are clearly not near the channel center, this does not affect the data analysis.

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} \cos\psi \cos\phi - \sin\psi \cos\theta \sin\phi & \cos\psi \sin\phi + \sin\psi \cos\theta \cos\phi & \sin\psi \sin\theta \\ -\sin\psi \cos\phi - \cos\psi \cos\theta \sin\phi & -\sin\psi \sin\phi + \cos\psi \cos\theta \cos\phi & \cos\psi \sin\theta \\ \sin\theta \sin\phi & -\sin\theta \cos\phi & \cos\theta \end{pmatrix}$$

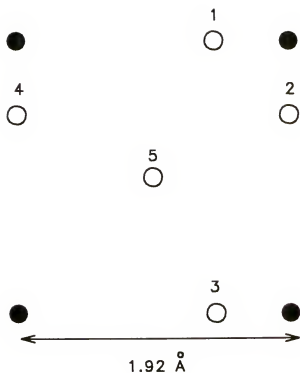


Figure 5-4. A single (100) channel showing how the site program works. Large black dots are silicon atom rows, and the open circles are various sites that the program must deal with. Site 1 is the inputted trial site, and site 2 is the rotated site obtained from a step. Sites 3 and 4 are included so as to properly account for the fact that sites 1 and 2 are partly outside the channel. Finally, site 5, an interstitial site, is in the same position when rotated and is fully enclosed in the channel, making correction sites unnecessary.

$$\times \begin{pmatrix} x_{100} \\ y_{100} \\ z_{100} \end{pmatrix} \quad (5-1)$$

Table 5-1. Coordinate transformations for axial directions. Angles are in degrees.

Axis	#	ϕ	θ	ψ
$\langle 100 \rangle$	1	0	0	0
	2	0	0	90
$\langle 110 \rangle$	1	45	-45	90
	2	-45	-45	-90
	3	135	-45	-90
	4	-135	-45	90

Overlap of Trial Positions with Monte Carlo Output

With the trial adsorbate coordinates in hand, we are now ready to overlap with the ion flux for a given crystal orientation (θ, ϕ) . We simply calculate the distance between the sites under consideration and the ions provided by the Monte Carlo program,

$$\text{dist} = \sqrt{(x_{\text{ion}} - x_{\text{site}})^2 + (y_{\text{ion}} - y_{\text{site}})^2}. \quad (5-2)$$

Thus, we only need the tranformed x and y coordinates (we can ignore the tranformed z coordinate), as it is essentially a 2D problem.

In order to calculate the weight that should be given to an overlapped ion, we introduce the idea of a 2D vibrational amplitude [Niel88a]. Atoms vibrate in 3D, of course, and in principle the vibrational amplitude in any dimension can be different from any other near the surface [Aler89], (u_x, u_y, u_z) , where u is the 1D RMS thermal vibration amplitude along the specified axis. Further, the vibration is generally taken to be gaussian about the atomic position in a given dimension. If one wanted to calculate the size of vibrations in the x-y (surface) plane, for example,

one might try $\sqrt{u_x^2 + u_y^2}$. If the vibrations are largely isotropic at least in the 2D plane that is being considered, then we can introduce the 2D vibrational amplitude $\rho = \sqrt{2}u$ (where u is the isotropic 1D vibrational amplitude). This is a parameter that must also be investigated in the simulations, as surface vibrations are not well understood [Wood86], and is inputted along with the adsorbate position. Thus, an overlapped ion can be weighted assuming that the adsorbate vibrates in two dimensions about its inputted site with a standard deviation equal to $\frac{1}{\sqrt{2}\rho}$, or,

$$\text{val} = \exp^{-(\text{dist}/\rho)^2}. \quad (5-3)$$

Val is then further scaled to take into account the energy dependence of the Rutherford scattering cross section (channeled ions can take on a wide range of exit energies). The energy of the ion is compared to the incident energy and val is modified accordingly,

$$\text{val} = \text{val} \times (E_0/E_{\text{ion}})^2. \quad (5-4)$$

Val is now added to the scattering yield and the process is repeated for all ions and all sites to obtain the total relative scattering yield for that crystal orientation. This is a tedious calculation. In order to speed it up, if dist is more than two 2D vibrational amplitudes away from the site, the addition to val for these ions is insignificant, so the calculation is not performed.

In addition to keeping track of the scattering yield, the energy distribution also provides indispensable information, and is available since we have the ion energies. After val has been scaled for the energy dependence of the cross section, the energy of the ion is multiplied by an appropriate kinematic factor. For Sb scattering into the 79° detector (this is the detector of choice, see Chapter 4), this value is

0.948. Any possible isotope effects (altering the kinematic factor) are small and are ignored. The resulting scattered ion energy must now be placed in an energy array, attempting to build up an energy distribution from the overlapped ion flux.

Basically, an energy array with a 2 keV bin width and covering a large enough energy difference is set up (2050-2450 keV is a typical energy range). A binary search is undertaken, whereby the array is divided into two equal parts. It is then determined into which half the scattered ion energy belongs. This smaller region is then divided into equal parts, and the process continued until the location of the energy on the array is found to better than 2 keV. Val is distributed to the two nearest array elements (assuming that the energy doesn't exactly match an array element) weighted by how close the actual energy is to that array element. Analogous to the scattering yield calculation, this is repeated for all ions and then all sites under consideration, resulting in a scattered ion energy distribution from a particular site(s). The energy distribution is smoothed to take into account straggling of channeled ions [Yang91] (actually calculated before scattering, see Chapter 3 and Chapter 6), and the detector resolution. The energy distribution is also normalized to an area of two by dividing by the calculated scattering yield.

Comparison of Simulation and Experiment

As all the above was for one crystal orientation, the procedure is repeated for all crystal coordinates under investigation by experiment. This results in a set of simulated scattering yields and energy distributions (already normalized to an area of two) for crystal coordinates that correspond to the experimental conditions for a single inputted trial site. The simulated scattering yields are now normalized so that the scattering yield for "random" incidence is one, and can be further corrected

as an input option to account for radiation induced desorption of the adsorbate(s) [Gran92]. We now directly compare the simulated and experimental data, as the experimental energy distributions and scattering yields have previously been reduced for just this purpose (see Chapter 4).

In order to evaluate how well simulation and experiment compare, we calculate a χ^2 value,

$$\chi^2 = \sum_i \frac{(N_i - n_i)^2}{n_i}, \quad (5-5)$$

where n_i is from the known distribution (the experimental data) [Pres92]. To calculate χ^2 , a simulated energy distribution is approximated by straight lines between successive points. Each point in the corresponding experimental distribution now has its vertical separation from the simulated distribution (joined by the line approximation) calculated. Thus, a value for χ^2 can be readily obtained for the fit. This is repeated for all of the simulated distributions, resulting in several χ^2 values. Further, a χ^2 value is calculated for the comparison of simulated and experimental scattering yields (in the form of yield versus tilt; an angular scan [Feld82]). Now we are ready to try other trial sites and see if the fit can be improved, eventually finding the adsorbate position on the surface.

Positions in the Surface Plane

Having obtained χ^2 values comparing experimental and simulated data, we can concentrate on trying to locate the adsorbate site on the Si(100) surface by minimizing χ^2 . The first step is to locate the adsorbate in the surface plane, ignoring, for now, the position normal to the surface. This can be accomplished by considering the experimental data for directions close to the $\langle 100 \rangle$ axis. Since these directions are almost normal to the surface, exiting ions will not be sensitive to the adsorbate

position normal to the surface as this position is along the direction of motion of the ions (see Figs. 5-1 and 5-2) and thus not sensitive to the channeling effect.

We next try adsorbate positions in the surface plane by varying the x coordinate(s) of the non-rotated dimer in the basic channel and obtaining χ^2 values. In principal, both x and y can be varied, but it is assumed that a dimer will not twist off the edge of a channel [Gran94b]. This information is sent to an output file, and a program, SORT.FOR [Bosh94d], finds the minimum χ^2 for either the scattering yield or the sum of all energy distributions. The “best fit” is identified based on adsorbate coordinates that yield low χ^2 values for both the scattering yield and energy distributions. These coordinates become the adsorbate position in the surface plane and are fixed.

In practice, the above procedure is accomplished by inputting a range of x coordinates to try and a total number of iterations. The program will then step through the inputted range with a step size determined by the number of desired iterations,

$$\text{stepsize} = (x_{\text{stop}} - x_{\text{start}})/(\text{iterations} - 1). \quad (5-6)$$

After a rough fit with a “large” step size has been completed, an x range with a finer step size can be performed and best x coordinate pinpointed. If two adsorbate positions have been inputted for asymmetric dimers, one or both x coordinates can be varied. Further, the step size for different sites needn’t be the same.

Table 5-2 shows sample input for the site program. The Monte Carlo program name determines whether the scan is a $\langle 100 \rangle$ (C18) or a $\langle 110 \rangle$ (C28) as the site program operates differently for the different axes. The Monte Carlo output files for a $\langle 100 \rangle$ scan are C18F.01, C18F.02, etc. (C18F.*), where C18F.01 is aligned

with the axis and the crystal orientation is for increasing tilt from the axis with increasing file number (for the $\langle 110 \rangle$ axis, file names are C28.*). The simulated energy distributions are C18L.* with the simulated scattering yields being C18L.ASM (experimental scattering yields are recorded in C18L.ADT, see Chapter 4). The χ^2 values for both energy distributions and scattering yields are outputted to the chi output file (along with the iterative site corresponding to these various χ^2 values), and this is the file on which SORT.FOR operates. The number of simulations is the total number of points in the angular scan, FWHM is the experimental energy resolution arrived at by a comparison of simulation and experimental energy distributions for “random” alignment, and calculation stop indicates when the ion is too far away to justify the calculation (two 2D vibrational amplitudes in this case). The kinematic factor (for Sb at 79°), and the scattering yield correction for desorption of the adsorbate have been mentioned. Finally, the start, stop, and number of iterations for x, y, and z coordinates as well as 2D vibrational amplitude are specified for each of the two possible inputted adsorbate sites.

Positions Normal to the Surface Plane

The $\langle 110 \rangle$ scan is used to probe adsorbate location normal to the surface, as the z coordinate was not needed for the $\langle 100 \rangle$ scan. The inputted z coordinate is used to transform the site positions for the $\langle 110 \rangle$ axis, and z can thus be probed using directions close to this axis. The x coordinate for the site(s) obtained from the $\langle 100 \rangle$ scan are not varied for this direction as the number of parameters would become too large otherwise. In addition, this direction is not the most sensitive to the x coordinate (as it is coupled with the z coordinate in the transformation).

Table 5-2. Sample input into the site program, SITE.FOR. Up to two inputted sites are possible.

Parameter	Value
Monte Carlo program name	C18
Monte Carlo input file name	C18F.*
Energy distribution output file	C18L.*
Chi output file name	100SB.C12
Number of simulations	9
FWHM for gaussian smoothing	25
Calculation stop	2
Kinematic factor	.9481830
Desorb slope	.00036
μ C per point	24
Include desorption? (yes=1)	0
2D vibrational amplitude start of site 1	.10
2D vibrational amplitude stop of site 1	.25
Number of iterations for 2D vibrational amplitude	11
X coordinate start of site 1	.200
X coordinate stop of site 1	.300
Number of iterations for X coordinate	11
Y coordinate start of site 1	.354
Y coordinate stop of site 1	.354
Number of iterations for Y coordinate	1
Z coordinate start of site 1	.000
Z coordinate stop of site 1	.000
Number of iterations for Z coordinate	1

The method of data analysis is then identical to that specified above, with the exception that z and not x is varied. Thus, when the “best fit” is obtained for this scan, x and z have been specified, y is assumed (no dimer twisting), and we have located the adsorbate site on the Si(100) surface (relative to the bulk atomic positions defining the basic channels, of course).

Adsorbate Vibrations

The parameter as yet not mentioned is the 2D vibrational amplitude. Indeed, although not indicated above, each angular scan must have two parameters varied. To reiterate then, the $\langle 100 \rangle$ data have the x coordinate and the 2D vibrational

amplitude of the adsorbate for these directions, ρ_{100} , to investigate, while the $\langle 110 \rangle$ data have the z coordinate and the 2D vibrational amplitude for these directions, ρ_{110} , to vary. If the adsorbate vibrations are completely isotropic, then the 2D vibrational amplitudes are the same. However, anisotropic surface vibrations are expected [Aler89]. Thus, the vibrational parameters must be varied independently between the two axes. This makes the data analysis more difficult, but it is not intractable, and much can be learned about the anisotropy of surface vibrations if the vibrations are varied independently. Typical resolution in atomic adsorbate position and vibrational amplitude using this method is $0.1 \text{ \AA}$, with the primary limiting factor being the extra parameters that the uncertain surface vibrations bring.

Site Program Test : Sb on Si(100)

This section describes in detail an experiment undertaken (Sb on Si(100)) to test the methodology described so far (based on our paper Ref. [Bosh95c]). Indeed, the experiment was chosen as the system is well studied and fairly simple as Sb is believed to form symmetric dimers on the Si(100) surface, providing fertile ground for the fine tuning and testing of our techniques. The data acquisition techniques of Chapter 4 and site program described above are extensively tested by examining this system. In addition, we investigate the energy loss model of Chapter 3 on a particular site. However, the results of this test experiment were not without surprises, showing the strengths of our methods. The following will detail the experiment and the findings, also giving an example of what has been discussed in Chapter 4 and so far in Chapter 5.

We describe the use of a fully tested Monte Carlo simulation [Dygo88; Dygo89; Dygo94c; Dygo94d] complete with a model for the impact-parameter dependent energy loss (applicable to MeV H and He incident ions) [Dygo94e; Dygo94f; Bosh95b] to study the system of Sb on Si(100)-2x1. This well-researched system was chosen primarily to investigate what the adatom energy distributions could offer in addition to the adatom yield versus tilt data. Angular scans were taken through the $\langle 100 \rangle$ and the $\langle 110 \rangle$ axes in silicon at azimuths where planar influences are minimal. The detailed energy distributions of ions scattering from the Sb adatoms as well as the scattering yield versus tilt from the high-index directions were compared with the Monte Carlo simulation. The “best fit” between the experiment and the Monte Carlo simulation was for an Sb site in good agreement with previously published sites for this system [Gran92; Rich90; Lyma95]. The primary benefit of using the energy distributions in this study concerns the adatom vibrations. Namely, a single isotropic vibrational amplitude does not give reasonable fits for the energy distributions for both angular scans. Further, the vibrational amplitudes do not agree with those obtained in the previous studies, even though the Sb site agrees. A possible explanation for this as well as what needs to be done in order to improve the overall technique of using the adatom energy distributions is discussed.

Experiment

A detailed description of the experimental setup is found elsewhere [Seib93]. Thin single-crystal silicon windows ($\sim 1 \mu\text{m}$ in thickness) within a thicker Si frame were produced using a dopant-selective etch [Cheu80a]. Typical window size was

about 5 – 7 mm, with a thickness variation over the window of $\sim 5\%$. The samples were then chemically prepared *ex situ* by the Shiraki technique, [Ishi86] and transferred to an Ultra-High Vacuum (UHV) sample preparation chamber (base pressure $\sim 5 \times 10^{-11}$ Torr). The protective oxide was desorbed from the sample to obtain the clean Si(100) surface using a heat lamp to heat the sample to 825°C. The pressure during the approximately ten minute oxide desorption did not exceed 1.5×10^{-9} Torr. The sample then gave rise to a sharp (2x1) Low Energy Electron Diffraction (LEED) pattern.

After desorbing the oxide, Sb was deposited on the sample from a boron nitride effusion cell held near 550°C. With the effusion cell shutter open, the chamber pressure rose to the low 10^{-8} Torr range. The sample itself was heated to $\sim 500^\circ\text{C}$ by irradiation with a thin Ta strip through a sapphire shield. The sample temperature was determined through a separate calibration run in which thermocouples were attached directly to a (different) silicon thin window. The sample was exposed to several monolayers of Sb to ensure saturation of the surface. In agreement with Ref. [Slij92], saturation coverage in this experiment was found to be 0.85 ML (1 ML = $6.78 \times 10^{14} \text{ cm}^{-2}$), determined by RBS and accurate to $\pm 10\%$. Finally, the sample was slowly cooled to allow annealing. The LEED pattern following Sb deposition was (1x1) with weak, diffuse 1/2 order spots and a low background.

The sample was next transferred under vacuum to a UHV ion scattering chamber (base pressure $\sim 5 \times 10^{-11}$ Torr), and placed on a two axis goniometer with a resolution of 0.02° . The goniometer is also equipped to allow motion parallel and perpendicular to the beam direction. This chamber is connected via differential

pumping to a 3.5 MV Van de Graaff accelerator, with pressures as low as 1×10^{-10} Torr typically maintained with beam on sample.

A beam of 2.5 MeV He^+ ions was produced and collimated to an angular divergence of 0.03° . The beam spot on the sample was about $1 \text{ mm} \times 1 \text{ mm}$, usually allowing five spots on any given sample (changed via motion perpendicular to the beam) for angular scans (see below). Crystal alignment was performed with the Sb on the beam-exit side of the sample, as shown in Fig. 5-5. The alignment for any direction in the crystal was achieved to a precision of $0.04^\circ - 0.06^\circ$ using the methodology of Ref. [Dygo93c]. This relatively poor alignment is due to the fact that sample transfers under UHV can move the goniometer [Seib93]. Reference directions were measured by viewing the transmitted beam on quartz at the end of the beamline. Full sample orientation can thus be performed very rapidly, normally taking about five minutes.

As the Monte Carlo program is set up to simulate ion trajectories near the $\langle 100 \rangle$ and the $\langle 110 \rangle$ axes, experimental angular scans were obtained near these axes. Angular scans were chosen based on Monte Carlo simulations (see below) that located “random” planes, or tilts out of axial directions that are largely free from planar influences. For a given crystallographic axis, angular scans were thus taken at a fixed azimuth ϕ in crystal coordinates from the $\{100\}$ plane ($\phi = 11^\circ$ for scans near the $\langle 100 \rangle$ axis and $\phi = 10^\circ$ for scans near the $\langle 110 \rangle$ axis), starting aligned with the axis, i.e. $(\theta, \phi) = (0, 11)$. The angular scan then tilted away from the axis as follows: $\theta = 0.1^\circ, 0.2^\circ, 0.3^\circ, 0.4^\circ, 0.6^\circ, 0.8^\circ, 1.5^\circ$, and 6.0° (5.0° from the $\langle 110 \rangle$ axis). Each point in the angular scan was collected for 12 μC of the integrated beam

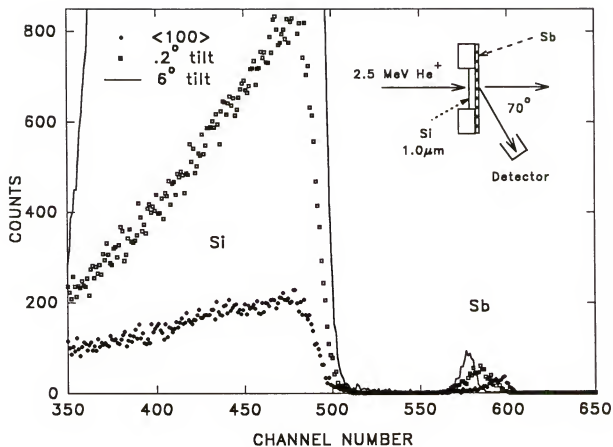


Figure 5-5. Energy spectra for 2.5 MeV He^+ ions transmitted through 1 μm thick Si crystal and scattered through 70° , taken aligned with the $\langle 100 \rangle$ axis, at a tilt of 0.2° , and at a tilt of 6.0° from the axis.

charge (obtained by a Faraday cup at the end of the beamline), attempting to minimize the scatter in the data from monolayer coverages of Sb and at the same time keeping possible irradiation damage in check (further minimized by aligning with the sensitive high symmetry directions first). Finally, as mentioned, the angular scans are not all performed on a single central beam spot, but each angular scan is performed on a single spot. A non-central spot potentially can allow the thickness variation of the sample to influence the data, since as the azimuth changes so does the exact beam spot, but different points in the angular scan involve small changes in angles, making such influences negligible.

Scattered ions were detected and energy-analyzed by three ion-implanted, passivated solid state detectors located at 70° , 78° , and 150° . The detectors in the transmission geometry had their energy axes calibrated indirectly using a thickness determination from the 150° detector (calibrated by backscattering) and the known energy loss associated with a “random” direction [Zeig77b]. For example, the direction $(\theta, \phi) = (6, 11)$ relative to the $\langle 100 \rangle$ axis can be considered a “random” direction (see below and Refs. [Dygo94f]). Energy distributions were then obtained from the Sb signal by dividing out the kinematic factor. Isotope effects were ignored.

Finally, a more precise sample thickness and the overall energy resolution were determined by requiring that the simulated distribution for the “random” direction matched the experiment. The energy resolution was found to be from 20–30 keV FWHM (experiment and detector dependent) and includes the detection system resolution, the energy spread of the incident beam, and the effect of sample nonuniformity. A linear background near the Sb signal was assumed and subtracted.

The energy distributions for different tilts were normalized to unit area, and the Sb scattering yields were normalized relative to the “random” yield.

Calculation of Site Dependent Energy Distributions

Energy Loss of Channeled Ions. The “best fit” impact-parameter dependent energy loss model was determined in these previous studies by direct comparison of simulation with experiment. For core electrons, the optimum fit was obtained using the semi-classical calculation [Kaba88] (raised by 12% from the theory). For valence electrons, the two-component free electron gas model using the solid-state valence electron density [Deut92] (decreased by 6% for both close and distant collisions) gave the best fit to the data. As pointed out in Ref. [Bosh95b], when aligned with the $\langle 110 \rangle$ axis or the $\{111\}$ plane, He^+ ions can remain in a non-equilibrium charge state for large penetration depths if well-channeled, making the energy loss model assumed inappropriate. However, as the angular scan in this study was not performed along a plane, and the Sb adatoms are not situated close to the channel center, ions interacting with these adatoms are likely to be properly accounted for under the above model.

We must further identify good “random” crystal orientations. Simulations using the energy loss model of Chapter 3 were performed at tilts of 6° from the $\langle 100 \rangle$ axis for azimuths between 0° (i.e. the $\{100\}$ plane) and 45° (i.e. the $\{110\}$ plane). Figure 5-6 shows the mean energy loss relative to the energy loss in an amorphous silicon target [Zieg77b] versus the azimuthal angle. Several high- and low-index planes are evident. Further, it is clear that the energy loss suffered by ions incident along the direction $(\theta, \phi) = (6, 11)$ differs negligibly from the amorphous target energy loss. Thus, by fixing $\phi = 11^\circ$ when tilting from the axial direction, one is

assured of an angular scan with minimal planar influence. A similar study near the $\langle 110 \rangle$ axis has been performed previously [Dygo94f]. This may seem somewhat restrictive. In principle, with a Monte Carlo simulation (unlike the continuum model approach), any azimuth may be simulated. However, the precision of our beam-sample system calibration is limited (see above). Therefore, by taking angular scans that minimize planar influences, we also hoped to minimize the effects of any errors in the beam-sample alignment (near planes, the energy loss and ion flux distribution is much more sensitive to small positional errors).

Site Dependent Scattering Yields and Energy Distributions. Using the Monte Carlo simulation complete with the impact-parameter dependent energy loss model described above, we are ready to simulate relative scattering yields and energy distributions of particular adatom locations within the channels. A large number of trajectories are followed by the Monte Carlo simulation, typically 20,000 for a given set of crystal coordinates corresponding to experimental crystal coordinates. This number of trajectories allows adatom sites that will interact with a small percentage of incident ions, *i.e.* near bulk-sites, to overlap with many ion positions. The position in the channel and energy of each ion after it has traversed the crystal is output. Figure 5-7 shows ion flux distributions at a few tilts from the $\langle 100 \rangle$ axis ($\phi = 11^\circ$ from the $\{100\}$). The highly non-uniform flux distribution is clearly seen for directions close to the axis, but rapidly smoothes out with tilts as small as $\sim 0.4^\circ$.

A trial adatom site is investigated by choosing a possible location in the channel. In addition, a trial 2D vibrational amplitude ρ can be assigned to the adatom, as surface vibrations vary substantially (factor of two or more) from bulk vibrations

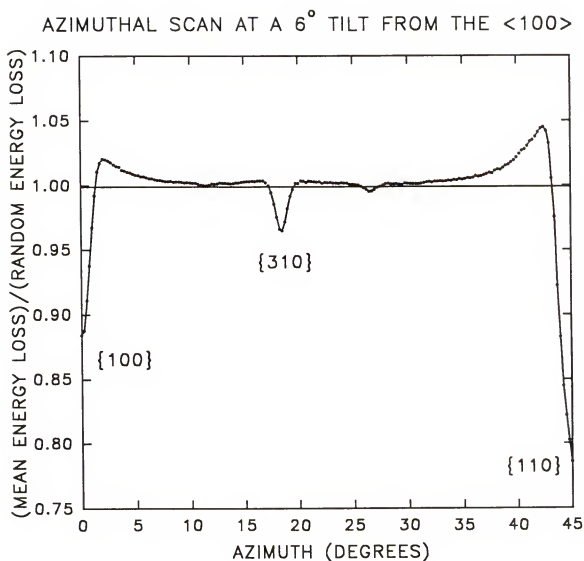


Figure 5-6. Monte Carlo simulated mean energy loss relative to random incidence energy loss at a tilt of 6.0° from the $\langle 100 \rangle$ axis for azimuths ranging from 0° (the $\{100\}$ plane) to 45° (the $\{110\}$ plane).

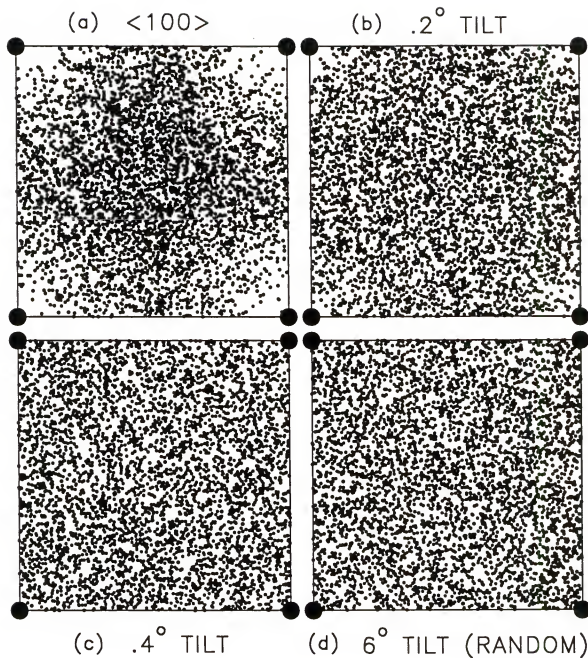


Figure 5-7. Ion flux distributions after penetrating $\sim 1 \mu\text{m}$ of a silicon crystal for four tilts (a) 0° , (b) 0.2° , (c) 0.4° , and (d) 6.0° from the $\langle 100 \rangle$ axis. Large black dots indicate atom rows.

[Wood86]. For a given set of crystal coordinates, the distance from the trial site to all of the outputted ions is calculated. If an ion is within four 2D vibrational amplitudes of the trial site (this includes virtually all of the ions able to scatter from the adatom), the gaussian centered at the trial site with a standard deviation equal to $\frac{1}{\sqrt{2}}\rho$ is evaluated for the ion distance and added to the scattering yield. This value is further scaled to take into account the energy dependence of the He-Sb scattering cross section. Simulated energy distributions are generated by binning the scattering yield value calculated above based on the energy of the ion. The resulting simulated energy distributions are smoothed to include energy straggling [Yang91] as well as the overall experimental energy resolution. This is done for all of the crystal coordinates investigated by experiment, resulting in a set of simulated scattering yields (normalized to the yield obtained at the furthest tilt from the axis, the “random” yield) and a set of simulated energy distributions (normalized to an area of unity) for a given trial site and trial vibrational amplitude.

Each simulated energy distribution is compared with the corresponding experimental distribution. With tilts close to the high symmetry direction weighted heavily compared to larger tilts (relative to χ^2 for zero tilt, small tilts are weighted by about half due to sample alignment uncertainty, and larger tilts about one-tenth or less as virtually all trial sites fit the data at near-random incidence), χ^2 is calculated for all of the fits together. Similarly, χ^2 is calculated between experimental and simulated relative scattering yields. For a trial site (and trial vibrational amplitude) to be considered a candidate for a true adatom position, both the total energy distribution fit and the relative scattering yield fit must have low χ^2 values and must look good visually.

As the $\langle 100 \rangle$ scan is not sensitive to adatom location normal to the surface, this scan is used to pinpoint adatom displacements from bulk positions in the surface plane. Also, the 2D vibrational amplitude ρ of the adsorbate in the plane of the surface is found with this scan. The best fit adatom position in the surface plane is fixed, and the $\langle 110 \rangle$ scan is then used to probe the adatom position and vibrational amplitude normal to the surface, as the sample is tilted by 45° for this scan.

Results and Discussion

The results of the data analysis described above are summarized in Figs. 5-8 and 5-9. As several studies on this system have reported the Sb adatoms to be in a modified bridge site (symmetric dimers) [Gran92; Rich90; Lyma95], this type of site was assumed for our study. Figure 5-8 shows the experimental Sb energy distributions aligned with the $\langle 100 \rangle$ and the $\langle 110 \rangle$ axes compared with a few selected trial site energy distributions (bumps in the simulations result from the limited number of trajectories followed), while Fig. 5-9 shows the experimental Sb yields versus tilt from the $\langle 100 \rangle$ and the $\langle 110 \rangle$ axes compared with the selected trial site yields versus tilt. Specific mention should be made of the fact that the theoretical value of the Sb dimer bond length ($\sim 2.93 \text{ \AA}$) [Tang93] does not produce a reasonable fit.

In comparing the solid line site to the other simulated sites displayed in Fig. 5-8, one notes that the solid line is not obviously the best reproduction of the experimental data. However, when considered together with the energy distributions at other tilts not shown, as well as with the simulated yield versus tilt in Fig. 5-9, the solid line becomes the optimum fit to the experimental data. To illustrate this more clearly, let us consider Figs. 5-8(b) and 5-9(b). In Fig. 5-8(b), the solid line

Figure 5-8. Simulated energy distributions obtained aligned with the (a) $\langle 100 \rangle$ and (b) $\langle 110 \rangle$ axes for trial Sb adatom sites and trial 2D vibrational amplitudes (DBL = dimer bond length, DFS = distance from bulk-extrapolated silicon surface).

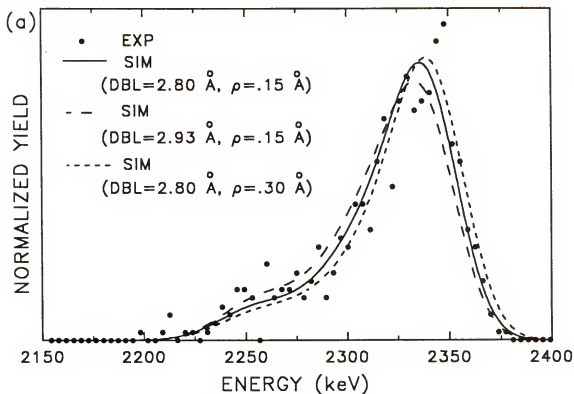
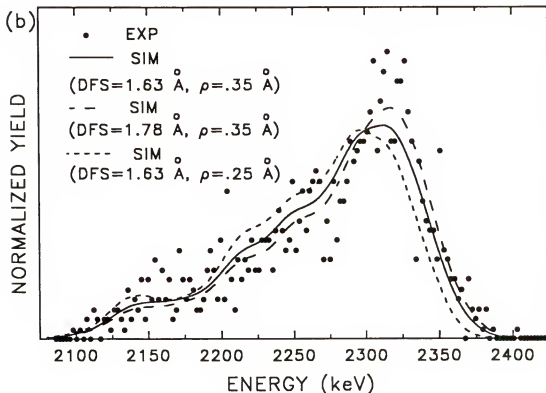
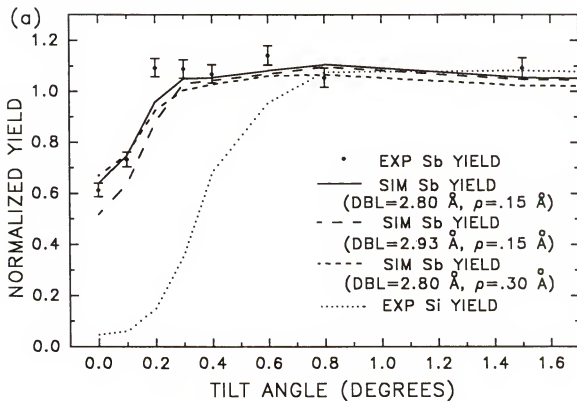
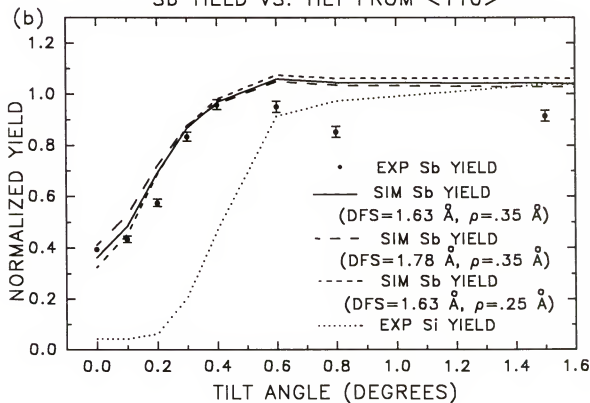
Sb ENERGY DISTRIBUTIONS $\langle 100 \rangle$ ALIGNEDSb ENERGY DISTRIBUTIONS $\langle 110 \rangle$ ALIGNED

Figure 5-9. Simulated scattering yield versus tilt from the (a) $\langle 100 \rangle$ and (b) $\langle 110 \rangle$ axes for trial Sb sites and trial 2D vibrational amplitudes (DBL = dimer bond length, DFS = distance from bulk-extrapolated silicon surface). The dotted line shows the experimental silicon yield.

Sb YIELD VS. TILT FROM $\langle 100 \rangle$ Sb YIELD VS. TILT FROM $\langle 110 \rangle$ 

represents a χ^2 value of about 0.19, while the long dash is somewhat higher (~ 0.25) and the short dash is about 0.17. This is because the short dashed curve fits the points in the tail (the majority of points) better than the other two curves. However, it fails to look good visually as the points around the peak are not very well reproduced. Indeed, none of the curves are able to fit the points around the peak remarkably well. It is possible to improve the fit visually in this region by increasing the vibrational amplitude (0.45 Å does nicely) but both χ^2 and the yield versus tilt fit suffer. Additionally, the χ^2 for all of the energy distributions together is lower for the solid curve. Turning to the yield versus tilt fits, Fig. 5-9(b), again the solid curve is not the lowest χ^2 (0.12 versus 0.11 for the short dashed curve and 0.14 for the long dashed curve). This is again somewhat misleading, as visually the solid curve passes close to more points than the short dash. Note that, as discussed below, these two curves (solid and short dash) are within our quoted experimental errors. Thus, χ^2 is useful for determining which fits should be looked at more closely, but a visual assessment is generally necessary as well. Indeed, the solid line in Figs. 5-8(a) (considering all the energy distributions) and 5-9(a) represents the lowest χ^2 value (i.e. 0.03 versus 0.05 for the short dash and 0.08 for the long dash in Fig. 5-9(a)) as well as the best visual fit. So, by a combination of χ^2 and visual fit to both energy distributions and yield versus tilt, we arrive at the solid curve as the “best fit”.

Further, by determining visually when χ^2 becomes too large to produce a reasonable fit, error bars on the measurement can be estimated. In this way, we can estimate the error bars for all results (including the 2D vibrational amplitude) to

be no larger than $0.10 \text{ \AA}$, the estimated error bars when using the continuum approximation [Seib93]. However, as mentioned in previously, improvement in this area can be made with more precise beam-sample alignment.

Figures 5-10 and 5-11 show the full set of experimental and best site simulated energy distributions for the $\langle 100 \rangle$ scan and the $\langle 110 \rangle$ scans, respectively. Note that small tilts ($\sim 0.2^\circ$) from the axial directions are the most sensitive to goniometer positional error, as ion flux distributions are changing rapidly. In the best fit dimer site, the Sb adatoms have a dimer bond length of $2.80 \text{ \AA}$, and reside $1.63 \text{ \AA}$ above the bulk-extrapolated Si surface plane. The Sb best fit site is shown in Fig. 5-12. Further, the best fit displays an anisotropic vibrational amplitude, as the 2D vibrational amplitude, ρ , parallel to the surface is $0.15 \text{ \AA}$ (based on the $\langle 100 \rangle$ scan), while when the sample is tilted by 45° , ρ jumps to $0.35 \text{ \AA}$ (based on the $\langle 110 \rangle$ scan).

These results are in agreement with several other studies of this system. Most recently, X-ray Standing Wave (XSW) measurements by Lyman *et al.* [Lyma95], have found data consistent with symmetric Sb dimers having a bond length of $2.81 \pm 0.09 \text{ \AA}$ and residing $1.64 \pm 0.02 \text{ \AA}$ above the bulk-extrapolated Si surface. This result agrees quite well with that of Grant *et al.* [Gran92], using transmission MeV ion channeling (the continuum approximation), who also found symmetric dimers with a dimer bond length of $2.8 \pm 0.1 \text{ \AA}$ and $1.63 \pm 0.07 \text{ \AA}$ above the bulk-extrapolated surface. Finally, a Surface Extended X-ray Absorption Fine Structure (SEXAFS) study by Richter *et al.* [Rich90], found a dimer bond length of $2.88 \pm 0.03 \text{ \AA}$, located $1.74 \pm 0.05 \text{ \AA}$ above the relaxed Si surface.

In light of the agreement in our Sb site with other studies, we may examine the Sb vibrations in a little more detail. Namely, given the above Sb site, the 2D

Figure 5-10. Simulated energy distributions for the “best fit” Sb site and 2D vibrational amplitude (see text) compared with experimental energy distributions for tilts from the $\langle 100 \rangle$ axis ($\phi = 11^\circ$).

<100> ANGULAR SCAN ENERGY DISTRIBUTIONS

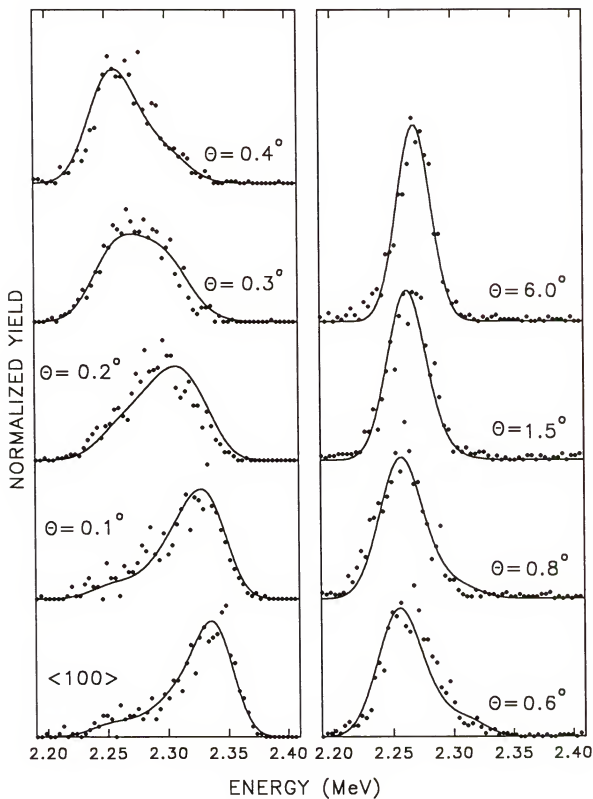
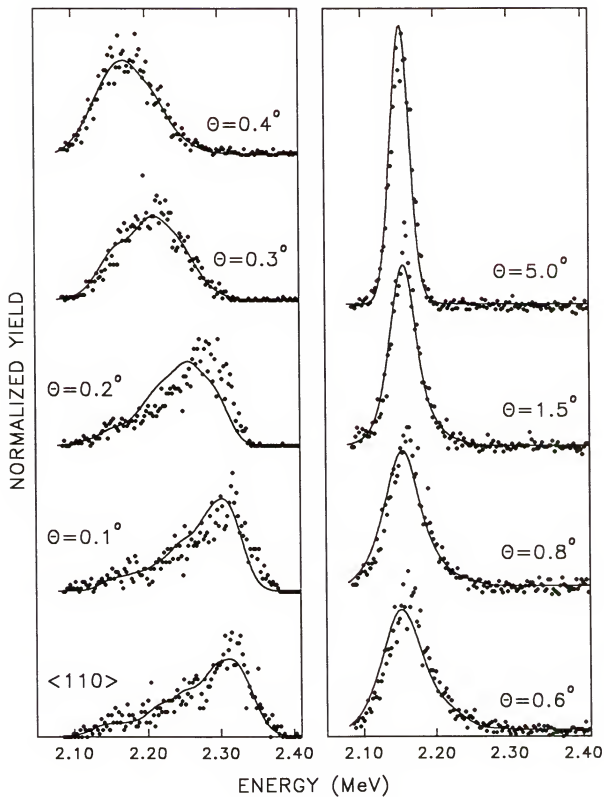


Figure 5-11. Simulated energy distributions for the “best fit” Sb site and 2D vibrational amplitude (see text) compared with experimental energy distributions for tilts from the $\langle 110 \rangle$ axis ($\phi = 10^\circ$).

<110> ANGULAR SCAN ENERGY DISTRIBUTIONS



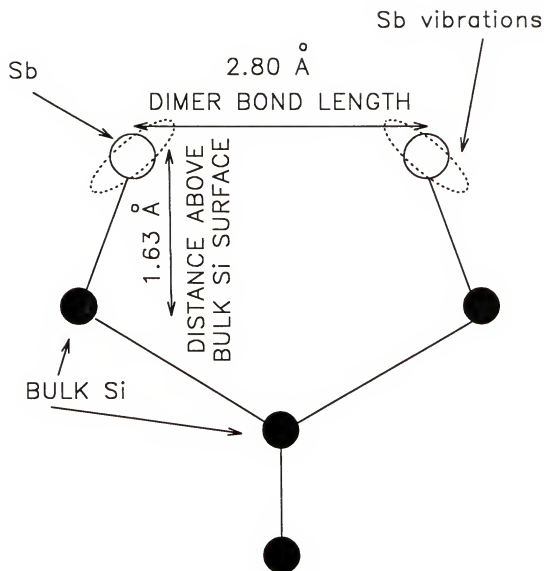


Figure 5-12. Details of the "best fit" Sb site. The view is along the $\langle 110 \rangle$ axis. The dotted ellipses show the proposed anisotropic Sb vibrations (see text).

vibrational amplitude, ρ , in the $\langle 100 \rangle$ scan cannot be raised above about 0.25 Å before the fits start to suffer noticeably. However, lowering ρ to 0.25 Å for the $\langle 110 \rangle$ scan can be ruled out (see Fig. 5-8). Thus, it would appear that the Sb adatoms are vibrating anisotropically. The ion channeling result [Gran92] claims that ρ should be isotropic and equal to 0.25 ± 0.1 Å, the average of the values found in this study; this result may be expected based on the similarity of the methods. However, XSW [Lyma95] suggests that the 1D vibrations normal to the surface should be smaller than our results imply, no more than 0.18 Å.

In order to reconcile the present results with this previous data, we can consider the possibility that the Sb adatoms vibrate primarily along their bonds (see Fig. 5-12). This would involve two Sb-Si bonds and the Sb-Sb dimer bond. By summing the vectors associated with these bonds (assuming the Sb-Si bond length of 2.63 Å [Rich90] as well as results found here), the largest Sb vibrations should occur tilted with respect to the sample normal by $\sim 45^\circ$. Since we can then expect that vibrations perpendicular to this principal vibrational axis will be relatively small, the vibrational amplitudes normal to the surface and in the surface plane will only be a component of the principal vibrations. This may result in smaller vibrational amplitudes both normal and parallel to the surface than at 45° (the $\langle 110 \rangle$ tilt angle), more in line with previous results.

CHAPTER 6 SURFACTANT-MEDIATED GROWTH OF Ge ON Si(100)

Modifications to Site Determination

In order to study more than one adsorbate on the surface, modifications to the site determination program discussed in Chapter 5 had to be made. “Heavy” adsorbates on the surface tend not to be separated very well in the energy spectra as the kinematic factors are not sufficiently different (see next sections). For example, the kinematic factors for Sb and Ge (adsorbates used in the following sections) scattering into 79° are .948 and .915 respectively. This compares with .793 for Si, which is well separated from the adsorbate peaks. The problem is that the site determination program described in Chapter 5 requires the individual peaks to be resolved so that the adsorbates can be simulated separately. This can be achieved for thin ($\sim 2000 \text{ \AA}$) Si windows using gaussian fitting programs to fit the adsorbate peaks, introducing additional uncertainty into the data analysis. Indeed, this has been done (using the continuum model of channeling) [Gran92a; Gran94c]. However, for thicker windows, the energy loss of channeled ions results in complex, non-gaussian, shapes in the energy distributions [Bosh95b], and the two peaks tend to blend together completely, making such peak extraction impossible. Thus, a new version of the site determination program was designed to allow the simultaneous simulation of two adsorbates, making individual peak extraction unnecessary.

There are three major things to take into consideration to accomplish this. First, one must consider the difference in scattering cross section between the two

species being considered. For example, the ratio for Sb and Ge scattering into 79° with an ion beam energy of 2.4 MeV (ion energy after penetrating a typical Si window) is 2.54 (Sb is more likely to cause a scattering event due to its larger atomic number). This ratio is rather insensitive to scattering angle and energy of the ion beam, indeed, at 2.3 MeV and 150° , the ratio is still 2.55. The program takes the cross section difference into account by dividing val (see Chapter 5) by 2.54 if the species currently under consideration is Ge, determined by inputting a species number for each inputted site, 1 for Sb or 2 for Ge.

Secondly, one must consider any difference in coverage between the two adsorbates. The coverage of the adsorbates is determined from the “random” spectrum (see Chapter 2). The resulting coverage ratio is maintained during the simulation by weighting the two adsorbates based on this ratio. Val is thus further adjusted to take this coverage difference into account.

The final consideration is the different kinematic factors of the adsorbates. Just before placing the energy of the ion in the energy array (see Chapter 5), the ion is multiplied by the kinematic factor for Sb if the species is 1, or the kinematic factor for Ge if the species is 2. Of course, any adsorbates can be used. One simply needs the cross section ratio and kinematic factors.

Thus, energy spectra involving multiple adsorbates can be generated with a few extra considerations. A few words should be said concerning yields. Yields from individual peaks are not possible as the peaks cannot be resolved (the reason for the above modifications). However, combined peak yields can still readily be obtained both by simulation and experiment. Combined peak angular scans are still possible then, but were abandoned for the following experiments (and taken out

of the site determination program) for the reasons outlined in Chapter 4 (discovered inaccuracy in beam-sample alignment). Instead of angular scans, a few interesting crystal orientations for each axis were examined that were insensitive to beam-sample alignment inaccuracies (see Chapter 4). Yields can still be used to normalize the energy distributions, if desired (see Chapter 4).

The number of possible inputted sites for the new program is five. This allows each adsorbate to occupy several possible sites. In addition, each possible site can be weighted differently from the others, as long as the total coverage ratio between the different adsorbates is maintained.

The focus of the data analysis had to change, however, because with complicated peak shapes involving two adsorbates mixed together, a comprehensive site determination is very difficult. One can generate any number of sites that fit the experimental data since so many parameters are now involved. The focus turned to using adsorbate sites found in the literature for simulation (either experimental or theoretical results, with slight variations allowed). Iterations over site positions are no longer necessary. The comparison between data and experiment is largely the same as that described in Chapter 5; χ^2 values are obtained between the energy distributions and used to distinguish between models proposed in the literature, and simulated combined peak yields for the models are directly compared with experimental combined peak yields (again, this yield comparison can be accomplished by normalizing the energy distributions to the random combined peak yield). Directions close to the $\langle 100 \rangle$ are favored as these directions give sites in the surface plane which most directly distinguish between sites proposed in the literature (positions normal to the surface plane do not play a major role in distinguishing models).

Further, surface vibrations have been found to be smaller (close to Si bulk values) in the surface plane than when the sample is tilted to the $\langle 110 \rangle$ axis [Bosh95c].

A final note concerns the calculation of straggling (see Chapter 3). Since straggling must be calculated before scattering (it is related to the amount of energy lost in traversing the crystal), temporary energy distributions must be set up for the two different adsorbates before multiplying by the proper kinematic factors. For example, the ions overlapping with Ge are used to build up an energy array separate from that for Sb. Straggling is then calculated for both of these temporary distributions, and then the distributions are multiplied by the corresponding kinematic factors, and combined into a single after scattering energy distribution.

Table 6-1 displays the input for the updated program. A fit to the experimental noise is added to the simulated energy distribution (see Chapter 4). An expected energy range is also inputted. Only one simulation is performed at a time, and the resulting energy distribution is sent to the energy distribution output file. The recent addition of unequal step types on the surface alluded to in Chapter 5 is included here as a percentage of step type 1 (the remainder being step type 2, the rotated step). Typically, this will remain a 50/50 ratio. The additional modifications discussed above are evident. Other parameters have been discussed in Chapter 5. Note that iterations over adsorbate positions are not performed. The following sections detail experiments performed using the modified site determination program presented here.

Ge and Sb Positions After Site Exchange

In this section, we examine the final stage of surfactant-mediated growth (necessary for a complete discussion of initial stages, see next section) through a study

Table 6-1. Sample input into the updated site program, SITE.FOR. Up to five sites are possible each with a different weight, and two different adsorbates are possible. Iterations are not performed in this version.

Parameter	Value
Monte Carlo program name	C18
Monte Carlo input file name	(C18F.)*
Energy distribution output file	EDIST.OUT
Chi output file name	ANSWER
Minimum energy expected	2000.
Maximum energy expected	2400.
Noise slope	-.000002
Noise intercept	.005
Number of simulations	1
FWHM for gaussian smoothing	23
Percentage of step type 1	50
Calculation stop	2
Kinematic factor for species 1	.9481830
Kinematic factor for species 2	.9145774
Cross section ratio for species	2.54
Weight of site 1	1
Species of site 1	1
2D vibrational amplitude for site 1	.15
X coordinate for site 1	.258
Y coordinate for site 1	.354
Z coordinate for site 1	.050

of the microscopic structure of the system Sb/Ge/Si(100) (Sb and Ge coverages $\sim 1\text{ML}$), where Sb is deposited first followed by Ge deposition at 350°C (based on our paper Ref. [Bosh96]). This should give a clear picture of what the system described in the next section would look like if the surfactant-mediated growth was allowed to complete, and where the participants would ultimately reside. The same system (but Ge deposited prior to Sb) was studied previously by Grant *et al.* [Gran94c], where adsorbate sites were identified using transmission ion channeling [Lyma91; Cheu81; Sten85; Gran92; Seib93] with angular scans and data were compared to a calculation based on the continuum model [Niel88a]. Here, we introduce the use of scattered ion energy distributions for site determination in a complex

system involving multiple adsorbates and sites. This new technique utilizes the fact that an adatom occupying a specific site within the channel interacts only with ions having particular trajectories, giving rise to particular energy losses of those ions, as they traverse the substrate crystal. Experimental energy distributions are thus compared to a Monte Carlo simulation of channeling [Dygo88; Dygo89; Dygo94c; Dygo94d] that includes a model for channeled ion energy loss [Dygo94e; Dygo94f; Bosh95b]. Our data are consistent with the sites found by Grant *et al.* A “naive” model of symmetric Sb dimers and substitutional Ge does not fit our data well.

Experiment

A detailed description of the experimental setup is found elsewhere [Bosh95c]. Thin single-crystal silicon windows ($\sim 0.18 \mu\text{m}$ in thickness) within a thicker Si frame were produced using a dopant-selective etch [Cheu80a]. A clean Si(100)-2x1 surface was obtained in Ultra-High Vacuum (UHV) by desorbing a “Shiraki oxide” [Ishi86]. After desorbing the oxide, Sb was deposited on the sample from a boron nitride effusion cell [Seib93]. The sample was held at $\sim 500^\circ\text{C}$ and exposed to several monolayers of Sb to ensure saturation of the surface, $\sim 0.85 \text{ ML}$ [Slij92] ($1 \text{ ML} = 6.78 \times 10^{14} \text{ atoms/cm}^2$). The Low Energy Electron Diffraction (LEED) pattern following Sb deposition was (1x1) with weak, diffuse 1/2 order spots and a low background. The sample was next placed in front of a Ge effusion cell. The sample temperature during the Ge evaporation was held at 350°C to ensure that the Ge/Sb layer attained its minimum energy configuration, without promoting Ge diffusion further into the bulk, as seen at higher temperatures [Sasa94]. The LEED pattern after Ge deposition was unchanged except for a slightly higher background. The Sb

and Ge coverages were 0.83 ML and 0.82 ML respectively, determined by Rutherford Backscattering (RBS) and accurate to $\pm 10\%$.

The sample was transferred under vacuum to a UHV ion scattering chamber (base pressure $\sim 5 \times 10^{-11}$ Torr) and placed on a two axis goniometer. The scattering chamber is connected via differential pumping to a 3.5 MV Van de Graaff accelerator. A beam of 2.5 MeV He^+ ions was produced and collimated to an angular divergence of 0.03° , resulting in a beam spot on the sample of about $1 \text{ mm} \times 1 \text{ mm}$. Crystal alignment was performed with the Ge/Sb on the beam-exit side of the sample, as shown in Fig. 6-1. In the transmission geometry, the low energy side of the Si peak corresponds to scattering from the beam-entrance side of the Si window. Thus, the Si surface peak in Fig. 6-1 occurs on the low energy side of the Si peak. Further, Sb can deposit on both sides of the thin Si window during evaporation, resulting in the two Sb peaks in Fig. 6-1. The submonolayer coverage of Sb on the beam-entrance side of the crystal (again, the low energy peak) does not affect the channeling of the beam, however.

Channeling directions involved in the experiment were found by viewing the transmitted beam on a piece of quartz at the end of the beamline. By monitoring the silicon yield and comparing with simulation, the accuracy of this procedure is estimated to be 0.02° – 0.05° . Channeling directions of interest can thus be found in a couple of minutes. Good approximations to “random” directions (necessary for adsorbate coverages, Si thickness, and overall energy resolution) were identified by simulation [Dygo94c; Dygo94c; Dygo94f], and the methodology of Ref. [Dygo93c] was used to locate these directions in the lab, making use of the reference directions found visually. Experimental energy distributions were obtained at three different

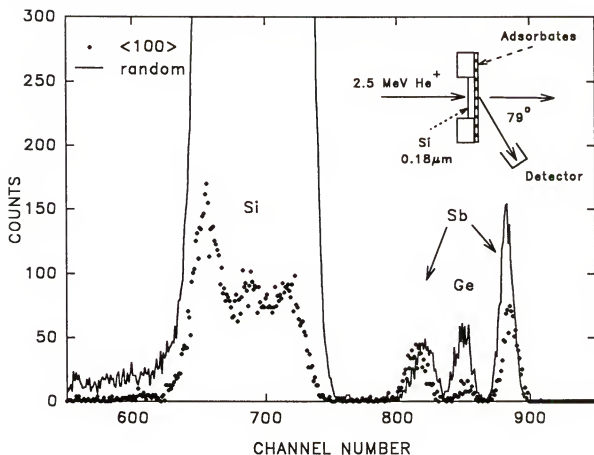


Figure 6-1. Energy spectra for 2.5 MeV He^+ ions transmitted through 0.18 μm thick Si crystal and scattered into a detector at 79°, taken aligned with the $\langle 100 \rangle$ axis (dots) and at a tilt of 6.0° from the axis in a “random” direction (solid line).

crystallographic directions, $(\theta, \phi)=(0,0)$, $(\theta, \phi)=(6,45)$, and $(\theta, \phi)=(6,30)$, where θ = tilt from the $\langle 100 \rangle$ and ϕ = azimuth relative to the $\{100\}$. These directions are, respectively, the $\langle 100 \rangle$ axis, the $\{110\}$ plane, and a direction found to be a good approximation to “random” incidence (directions where energy losses are close to those in amorphous media [Zieg77b]).

Scattered ions were detected and energy-analyzed by three ion-implanted, passivated solid state detectors located at 70° , 79° , and 150° . Energy distributions after scattering (the kinematic factor was not divided out) for the Ge/Sb signal were thus obtained. The energy distributions were each collected for $24 \mu\text{C}$ of the integrated beam current (high symmetry directions taken first to minimize irradiation damage) and all three were taken on the same beam spot to minimize adsorbate coverage and Si thickness variation. Finally, the energy distributions were normalized to unit area.

The Monte Carlo simulation program and how it can be used to create adsorbate site energy distributions (as well as advantages of using energy distributions) is described elsewhere [Bosh95c]. Briefly, a large number of ion trajectories are followed by the Monte Carlo simulation, typically 20,000 for a given set of crystal coordinates corresponding to the experimental conditions. In order to obtain the exit energies of the ions, a model for channeled ion energy loss is required. For this, we made the usual assumption that core and valence electrons contribute independently to the stopping. For the stopping due to core electrons, we employed the semi-classical approximation, and for stopping due to valence electrons, we used

the two-component free electron gas model [Dygo94e; Dygo94f; Bosh95b]. The position in the channel and *energy* of each ion after it has traversed the crystal are then outputted.

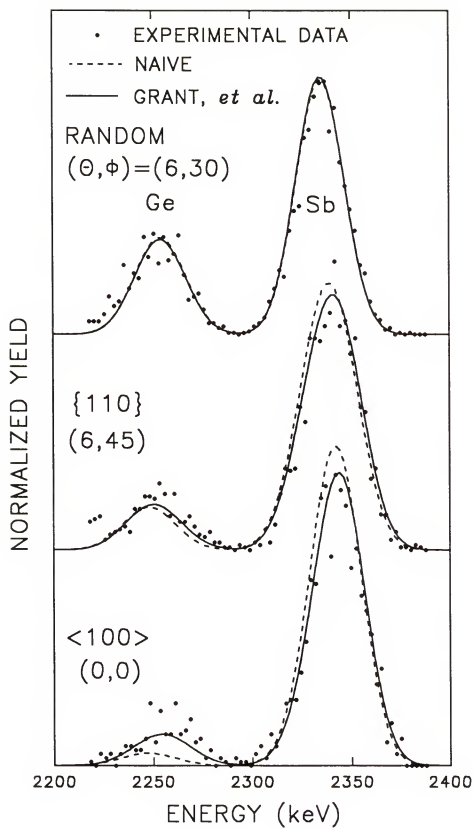
An adatom site can now be investigated by choosing a location in the channel. A 2-D vibrational amplitude, ρ , must also be assigned to the adatom ($\rho = \sqrt{2}u$, where u is the 1-D vibrational amplitude). For a given set of crystal coordinates, the distance from the trial site to all of the outputted ions is calculated. If an ion is within two 2-D vibrational amplitudes of the trial site, the gaussian centered at the trial site with a standard deviation equal to $\frac{1}{\sqrt{2}}\rho$ is evaluated for the ion distance and added to the scattering yield. This value is further scaled to take into account the difference between and energy dependence of the He-Ge/Sb scattering cross sections. Simulated energy distributions are generated by binning the scattering yield value calculated above based on the energy of the ion after scattering (the energy of the ion is multiplied by the kinematic factor of Ge/Sb for a given scattering angle). This is repeated for all sites (possibly involving several different adsorbates) under investigation. The resulting simulated energy distributions are smoothed to include the experimental energy resolution and straggling. This is done for all of the crystal coordinates investigated by experiment, resulting in a set of simulated energy distributions (each normalized to an area of unity) for a particular set of adsorbate sites and 2-D vibrational amplitudes. However, based on previous work where adsorbate vibrations were found to be only slightly enhanced from bulk vibrations in the surface plane [Bosh95c], ρ was set to 0.15 Å for both adsorbate species and not varied.

This resolution is achieved by comparing each simulated energy distribution with the corresponding experimental distribution and a χ^2 value of the fit is obtained. By varying the adatom positions, a best fit and most likely position for the adsorbates can be found. However, distributions near the $\langle 100 \rangle$ axis taken in this work are only sensitive to displacements from bulk positions in the surface plane as the $\langle 100 \rangle$ axis is along the sample normal. Thus, the goal of this work is to generate energy distributions of Ge/Sb sites found in the literature and to compare them with the experimental data.

Results and Discussion

Figure 6-2 summarizes the findings in the present work. The experimental data (dots) are compared with two models for the Ge/Sb system for the three energy distributions taken. It should be noted that the data are inconsistent with the Ge occupying any positions other than near-substitutional. This provides immediate evidence that the Sb has indeed floated to the surface, allowing the Ge to occupy near-bulk Si lattice positions underneath (allowing layer-by-layer growth). Thus, both models under consideration assume that the Sb has returned to the surface and that the Ge occupies near-substitutional positions underneath. The first model, a “naive” approach to the system, assumes the Ge has taken exactly substitutional positions and the Sb has dimerized symmetrically as if it were on the Si(100) surface (dashed line) [Gran92]. The second model is taken from Grant *et al.* [Gran94c] and places the Ge in asymmetric near-substitutional positions, while finding that the Sb dimer is also asymmetric with a tilt of about 7° . This site is illustrated in Fig. 1-2 (viewed along the sample normal).

Figure 6-2. Monte Carlo simulated energy distributions (lines) for possible Sb and Ge sites for the system Sb/Ge/Si(100) (see text) compared with experimental data (dots) for directions close to the $\langle 100 \rangle$. Note that all spectra are normalized to have the same area under the curve.



It can be seen from Fig. 6-2 that the “naive” model is not well reproduced by the experimental data. The Ge peak in this model is suppressed and shifted to too low an energy when aligned with the $\langle 100 \rangle$ axis. However, the energy distribution shape for the Grant model reproduces the experimental data quite well when aligned with the $\langle 100 \rangle$ axis as well as aligned with the $\{110\}$ plane.

Although a complete site determination of this system using energy distributions would require more data (off normal axes would have to be investigated to get adatom displacements along the sample normal), much can be inferred from the energy distributions in Fig. 6-2 alone. Namely, at least some of the Ge adatoms are located in sites slightly displaced from bulk ($\sim 0.4 \text{ \AA}$) with the Sb dimer residing above. This is perhaps not too surprising as subsurface reconstructions (often difficult to measure due to interference from the bulk signal) have been calculated to be from ~ 0.1 to $0.4 \text{ \AA}$ for Si subsurface layers [Trom83; Robe90; Jaya93], and Ge introduces some additional strain with its lattice mismatch. Further, the fact that the present data are consistent with the findings of Grant *et al.* is interesting in that in the present experiment, the Sb floated to the surface, as opposed to being deposited on top of the Ge. We thus find that the order of deposition under the present conditions does not significantly affect the preferred final sites of the adsorbates.

Ge and Sb in the Early Stages of Surfactant-Mediated Growth

The basics of surfactant-mediated growth and the benefits of the resulting layer-by-layer growth that can be achieved using this method have been discussed in Chapter 1. However, the microscopic details of the site exchange processes between Ge/Si and the surfactant are not well-understood, and in fact are debated

in the literature [Trom92; Yu94a; Ohno94; Yu94b]. Several models are available in the literature describing differing means by which the Ge/Sb site exchange occurs. Actually, the models discussed here are for As on Si(100), and we are considering Sb. As and Sb can be expected to behave in the same way here as (locally) they dimerize similarly on Si(100) (differences in behavior are readily attributable to the size difference of As and Sb) [Noga91]. One model due to Tromp and Reuter [Trom92] (referred to as the Tromp model) states that Ge arriving at the surface initially breaks the Sb dimers, forming rotated Ge dimers. As additional Ge dimers form in adjacent sites, a “two-dimer correlated exchange” occurs with the Sb. The total energy calculations of Yu and Oshiyama [Yu94a] (Yu model) describe a complex series of stages in which near-interstitial Sb is predicted, eventually leading, with a sufficient Ge coverage, to Sb on the surface. The final state itself, with Sb dimers on the surface and Ge in near-bulk sites (final state), has been determined experimentally [Gran94c; Bosh96]. In order to determine which path that the Ge/Sb site exchange follows, one must prepare the system in its initial bonding state. This may be done using a low Ge coverage since the models suggest that a locally high Ge concentration is necessary for the transition to the final state. Further, energy and diffusion barriers may be exploited to freeze the system in its initial state by deposition at room temperature. These barriers can then be explored by annealing the sample to see if a transition to the final state can be observed.

In this section, we examine the microscopic site exchange mechanism that occurs in surfactant-mediated growth through a study of the system Ge/Sb/Si(100) (Sb coverage ~ 1 ML, Ge coverage 0.15 and 0.68 ML). The Sb was deposited first, followed by Ge at RT. Experimental scattered ion energy distributions were obtained

for directions close to the $\langle 100 \rangle$ axis (the surface of interest on the beam-exit side of the crystal). A Monte Carlo simulation of channeling [Dygo88; Dygo89 Dygo94c; Dygo94d; Dygo94f; Bosh95b] was employed for the calculation of ion positions and energies as they exit the crystal. Simulated energy distributions were then calculated by taking adsorbate site locations from the literature and overlapping them with these ion positions (and corresponding energies). The experimental energy distributions were compared to the simulated energy distributions obtained for predictions of the adsorbate sites prior to the final site exchange [Trom92; Yu94a] as well as to a model for the final state configuration [Gran94c; Bosh96]. The sample was then annealed at 350°C for 10 min to see if energetics and diffusion would lead to site exchange. The data before annealing are consistent with undisturbed Sb dimers on Si, with Ge in loosely bonded dimers, whereas after annealing, for the 0.68 ML Ge coverage, the final state fits the data best, showing the importance of energetics in surfactant-mediated growth.

Experiment

A description of the experimental setup can be found elsewhere [Bosh96]. Sb was deposited on the clean, single-crystal Si window ($\sim 0.5 \mu\text{m}$ in thickness and 5–7 mm in diameter) from a boron nitride effusion cell [Seib93]. The sample itself was held at $\sim 500^\circ\text{C}$ and exposed to several monolayers of Sb to ensure saturation of the surface, ~ 0.85 ML [Slij92] ($1 \text{ ML} = 6.78 \times 10^{14} \text{ atoms/cm}^2$). The sample was then cooled to RT and placed in front of a Ge effusion cell, with an evaporation rate of $\sim 0.15 \text{ ML/min}$. The Sb and Ge coverages were 0.80 ML and (0.15 ML and 0.68 ML) respectively, determined by Rutherford Backscattering.

The sample was transferred under UHV to an ion scattering chamber (base pressure $\sim 5 \times 10^{-11}$ Torr) and placed on a two axis goniometer. A beam of 2.5 MeV He^+ ions was produced by a 3.5 MV Van de Graaff accelerator and collimated to an angular divergence of 0.03° . Crystal alignment was performed in a transmission geometry, with the Ge/Sb on the beam-exit side of the sample, “by eye” by viewing the transmitted beam on a piece of quartz at the end of the beamline. By monitoring the Si yield and comparing with simulation, the accuracy of this procedure is estimated to be 0.02° – 0.05° . Good approximations to “random” directions (directions where energy losses are close to those in amorphous media [Zieg77b]) were found as in Ref. [Bosh95c]. Experimental energy distributions were obtained at three different crystallographic directions, $(\theta, \phi) = (0^\circ, 0^\circ)$, $(\theta, \phi) = (6^\circ, 45^\circ)$, and $(\theta, \phi) = (6^\circ, 30^\circ)$, where θ = tilt from the $\langle 100 \rangle$ and ϕ = azimuth relative to the $\{100\}$. These directions are, respectively, the $\langle 100 \rangle$ axis, the $\{110\}$ plane, and “random” incidence.

Scattered ions were detected and energy-analyzed by three ion-implanted, passivated solid state detectors located at scattering angles of 70° , 79° , and 150° . The energy distributions were each collected for $24 \mu\text{C}$ of the integrated beam current. All three were taken on the same beam spot to minimize adsorbate coverage and Si thickness variation, and in order to minimize irradiation damage, the high symmetry directions were taken first. Finally, the energy distributions were normalized to the random yield. After collecting data for the three crystallographic directions described above, the sample was annealed at $\sim 350^\circ\text{C}$ for 10 min. Energy distributions as above were then obtained on a new beam spot. The Monte Carlo simulation program and how it can be used to create adsorbate site energy distributions is described elsewhere [Bosh96; Bosh95c]. A linear background (fit to

the experimental data) was assumed and added to the simulated energy distributions.

Results and Discussion

As discussed earlier, several models have been proposed for the initial stages in surfactant-mediated growth. The final state [Gran94c] is the experimentally determined Ge and Sb sites after the Sb has floated to the surface, incorporating the Ge into the bulk (Fig. 6-3(d)). The Tromp model offers a possible initial bonding state in which Ge arriving at the surface initially breaks the Sb dimers, forming rotated Ge dimers (Fig. 6-3(c)). At 0.15 ML coverage and assuming random Ge dimer site occupation, 80% of the Ge should not be able to undergo the “two-dimer correlated exchange” and the surface would be expected to be in this initial state. For 0.68 ML Ge coverage, the Tromp model would predict essentially all of the Ge to be in the final state. Note that the Tromp model assumes deposition at elevated temperatures and that the transition to the final state is driven by Ge coverage. Finally, the Yu model finds that Ge dimers bond initially between the Sb dimer rows (Yu model B, named for the figure in their publication, Fig. 6-3(a)). They refer to this configuration as stable, but contend that it is energetically favored to pass to a state in which the Ge and Sb exchange sites, resulting in interstitial Sb dimers between the Sb dimer rows and subsurface Sb-Ge dimers (Yu model C, Fig. 6-3(b)). Again, increasing Ge coverage facilitates a transition to the final state. Another model due to Ohno [Ohno94] would appear similar to the Tromp model in our technique.

For each of the above models, energy distributions for directions close to $\langle 100 \rangle$ were simulated and compared with the experimental data. In simulating these

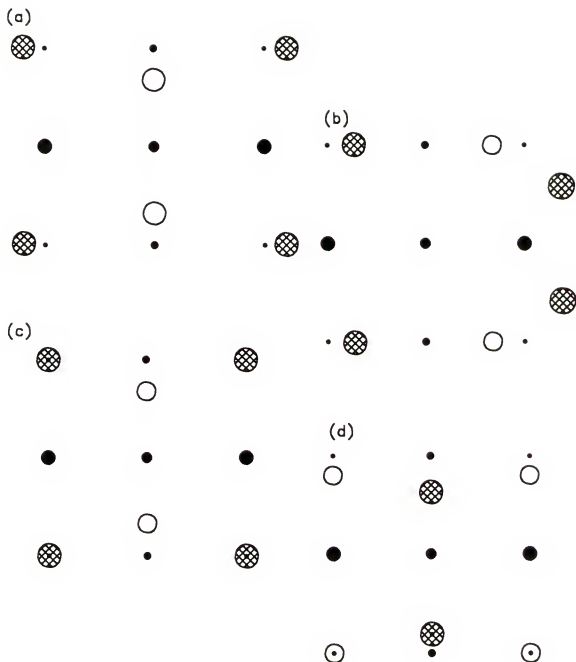


Figure 6-3. View of the Si(100) surface from above showing the models tested in the paper: (a) Yu model B (Ge dimers between weakened Sb dimer rows), (b) Yu model C (interstitial Sb atoms), (c) Tromp model (Sb dimers broken by Ge), and (d) the experimentally determined final state. Black circles represent Si, with the size indicating proximity to the surface, open circles are Ge and crosshatched circles Sb.

models, the exact choice of adatom location is somewhat uncertain as they are not all well-specified in the models (this excludes the final state which has experimentally determined sites). Coordinates had to be chosen for the adsorbates that would represent the models as closely as possible. For Sb dimerized with Sb or Ge, the channel position selected was the experimentally determined site for Sb dimerized with Sb on Si(100) [Bosh95c]. For Ge dimerized with Sb or Ge, the experimentally determined site for Ge dimerized with Ge on Si(100) without a tilt was used [Gran94b]. The interstitial Sb atoms in the Yu model are specified. Further, substitutional-like atoms in the models were assumed to be exactly substitutional. This is perhaps unlikely (subsurface reconstructions are expected [Trom83; Robe90; Jaya93]), but displacements up to $0.4 \text{ \AA}$ from bulk sites were tested and not found to affect the conclusions. Finally, for each Ge coverage, excess Sb was assumed to be dimerized on Si(100) in the usual manner.

Figure 6-4 displays before and after annealing $\{100\}$ axial aligned experimental data for 0.15 ML Ge coverage and how they compare with the final state (long dash line), the Tromp model (short dash), and Yu model C (medium dash). Based on these fits alone, it is clear that neither the Tromp model nor Yu model C fit the data well for either temperature. The same conclusions were evident for the $\{110\}$ planar data, not shown (all models, of course, fit the random distributions). The final state provides a better fit in both cases. Thus, either the final state is already present at 0.15 ML Ge coverage and RT, which would contradict both the Tromp and Yu models, or an initial state not yet investigated is present.

In Fig. 6-5, we show the data for a Ge coverage of 0.68 ML (Sb coverage unchanged). Again, neither of the discussed models fit the experimental data (nor

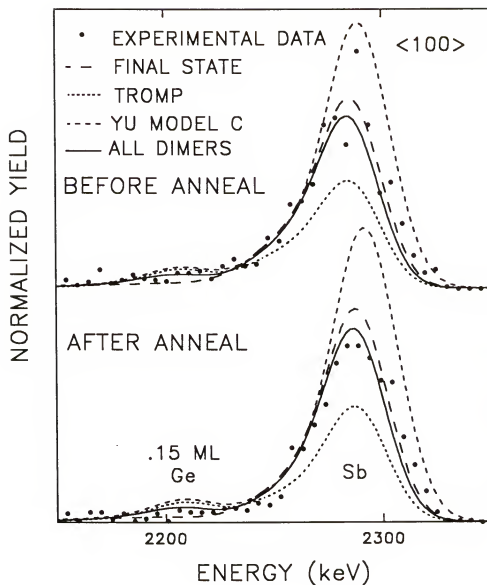


Figure 6-4. Monte Carlo simulated scattered ion energy distributions (lines) for possible Ge and Sb sites for the system Ge/Sb/Si(100) (see text) compared with the experimental data (dots) for the $\langle 100 \rangle$ aligned direction (both before and after annealing). The Ge coverage is 0.15 ML. All spectra are normalized to the random yield. Slight differences in simulations between before and after annealing are due to separate simulations for the different Si thicknesses (different beam spots).

would they be expected to at this Ge coverage). After annealing, (but not before) the final state fits both peaks extremely well, showing a clear transition from some intermediate state to the final state. The solid curve represents a simple model where the Sb dimers on Si(100) [Bosh95c] remain unbroken (and unaltered) when Ge is deposited. This model fits the unannealed Sb data very well. Further, for the unannealed case, if the Ge is assumed to dimerize on the surface, the same (surface plane) dimer bond length as Sb on Si(100) ($2.80 \text{ \AA}$) gives a good fit to the Ge data as well. We shall refer to this model as the all dimer model. It should be pointed out that the Ge need not actually dimerize, it must only be located in sites (relative to bulk sites) that mimic dimerization. Further, it is interesting that this model is similar to Yu model B. When Ge initially hits the surface, Yu, *et al.*, predict Ge dimerization between the Sb dimer rows accompanied by a weakening of the Sb dimers. However, we observe no weakening of the Sb dimers (would expect a lengthening of the Sb dimer), and the Ge site that they propose does not fit the data shown in Fig. 6-5 (dimer bond length is too short). Based on our experimental data, it appears that the all dimer model is a metastable initial state that can readily undergo a transition to the final state upon annealing.

We are now in a position to test this model in our low Ge coverage data. Returning to Fig. 6-4, we see that the all dimer model (solid line) competes very well with the final state. If this all dimer initial state offers a convincing fit to the data at high Ge coverage, then it would be expected to be present at low Ge coverages, and this is consistent with our unannealed data. In Fig. 6-4, it is not clear that a transition to the final state has occurred after annealing. The Ge data support a transition, however, the statistics are poor. Perhaps, as suggested by

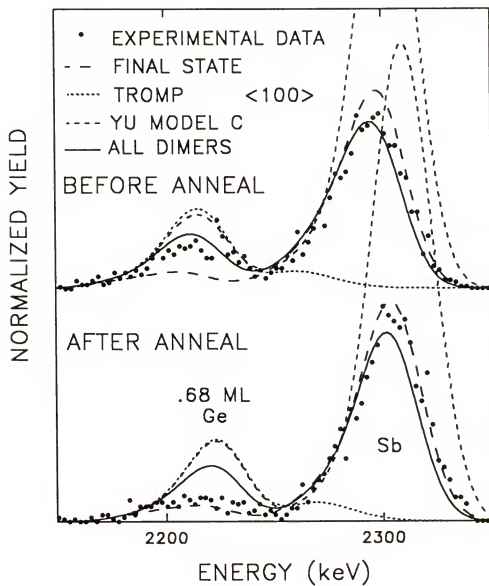


Figure 6-5. Same as Fig. 6-4, but Ge coverage is 0.68 ML.

both the Tromp and Yu models, at low coverage the transition to the final state is kinetically prohibited. Note also that the final state model in Fig. 6-4 corresponds to full ML Ge coverage. Small islands of Ge in the final state may give slightly altered positions from those assumed, possibly explaining a poor fit [Ohno94].

CHAPTER 7 CONCLUSIONS

Channeled Ion Energy Loss

Based on the comparison between experimental and Monte Carlo simulated energy-loss distributions for 625 keV H^+ ions transmitted through thin Si single crystals, it has been found that the impact-parameter dependence of the ion energy loss must include a role for distant collisions with core electrons in the stopping process. The stopping can be well described by the SCA model applied to core electrons and the 2-component FEG model applied to valence electrons. These models, based on first-order perturbation theory, reproduce very closely the extensive set of experimental distributions corresponding to detailed angular scans through axial and planar channels in Si, if a small adjustment of the stopping cross sections due to core and valence electrons is made. The corrections found, however, do not appear consistent with the current estimates of the contribution to the stopping due to the higher-order terms in the perturbation series.

The dependence of the energy loss to core electrons on the impact parameter, predicted by the SCA model, can be surprisingly well approximated by the MEEA model with the parameter $\Omega = 1.4$. Therefore, at least in distant collisions of the ion with core electrons, the mean excitation energy is about 1.4 times greater than the binding energy for a given shell. It has also been found that the local density approximation of Lindhard and Winther applied to valence electrons does not agree with the experimental data as well as the 2-component FEG model does.

The comparison between the solid-state and free-atom valence electron densities has shown a rather unexpected insensitivity of the energy distributions to the solid-state effects in the electron density in Si.

Further, the comparison between experimental and Monte Carlo simulated energy distributions for 2.5 MeV He^+ ions incident near the $\langle 100 \rangle$ and $\langle 110 \rangle$ axes in silicon shows that the above model of energy loss describes the stopping for this system as well. Namely, the SCA model for core electron stopping (cross section raised by 12% from theory) and the 2-component FEG model for valence electron stopping (cross section reduced by 6% from theory and using the solid-state electron density) provide an energy loss model that again reproduces the data throughout detailed angular scans around major axes in silicon, showing its validity over a wide range of impact parameters. However, the first order perturbation calculation assumes a fully stripped ion after entering the crystal. Indeed, systematic deviations are observed for directions close to the $\langle 110 \rangle$ axis in silicon, and these deviations can be explained if well-channeled He^+ incident ions are penetrating deep into the crystal before becoming fully stripped, suffering reduced stopping compared to the theory.

Site Determination of Sb on Si(100)

A Monte Carlo simulation of channeling that includes a tested model for channeled ion energy loss has been used for the site determination of Sb on Si(100). This allows both simulated scattering yields and energy distributions at tilts from high symmetry directions in silicon to be calculated for trial adatom sites. The inclusion of the energy distributions improves sensitivity to vibrations of the adsorbate. Further, through more precise beam-sample alignment, the energy distributions may

well be able to pinpoint adatom sites to better than $0.10 \text{ \AA}$ normally achieved using transmission ion channeling.

The Sb location found using the simulated scattering yields and energy distributions was in agreement with previously published experimental results on this system. However, the Sb vibrations showed some discrepancy. In order to fit the energy distributions close to the $\langle 110 \rangle$ axis, an enhanced 2D vibrational amplitude over previously published values had to be assumed for that direction. Thus, it would appear that the Sb adatoms vibrate preferentially along a $\sim 45^\circ$ diagonal with respect to the surface normal, implying smaller normal and parallel to the surface plane vibrational amplitudes. Such an explanation would bring our results into reasonable agreement with published values.

Surfactant-Mediated Growth of Ge on Si(100)

In conclusion, the microscopic site exchange mechanism for the complex system Ge/Sb/Si(100) responsible for surfactant-mediated growth (*i.e.* the transformation to Sb/Ge/Si(100) with the Ge occupying near-bulk sites) has been studied using scattered ion energy distributions. To isolate the system prior to the final site exchange, a low coverage of Ge was deposited at near room temperature. Experimental energy distributions were obtained for directions close to the $\langle 100 \rangle$ axis. A Monte Carlo simulation of channeling loss was employed for the simulation of energy distributions for predictions of several early stages in the site exchange process found in the literature.

It is found that an initial state similar to one proposed by Yu and Oshiyama (Yu model B) fits the data. We find, however, that room temperature deposition of Ge does not break or alter the Sb on Si(100) dimers, and the Ge itself is registered

with the substrate, possibly in loose dimers with about the same dimer bond length as the Sb dimers. After annealing, the best fit to the data for 0.68 ML Ge coverage is consistent with Sb returning to the surface, incorporating Ge into the bulk, indicating the role of energetics in surfactant-mediated growth.

Further, the microscopic structure of this system at high (1 ML) Ge coverage and Ge deposited at 350°C was also studied. From these studies, it is evident that the Ge atoms occupy near-substitutional (~ 0.4 Å from substitutional) sites, giving clear indication that the surfactant again resides on the surface. The location of all adatoms is in agreement with Grant *et al.* [Gran94c], indicating that depositing Sb before or after Ge does not greatly affect the final geometry.

APPENDIX A OXYGEN BEAM IMPURITY

A problem of some concern was noticed during a series of experiments. An unexpected peak sometimes manifested itself when Au was present on a sample. Figure A-1 displays this peak between the usual Si and Au signals for He backscattering. Further, the peak size varied with the amount of Au deposited on the sample; the more Au present, the larger the peak. It was then thought that the peak was an impurity in the Au that was being deposited. However, the peak location (for helium scattering) did not correspond to any reasonable impurity that might be present in Au. An attempt to identify a possible beam contaminant was then undertaken. A beam contaminant would explain why the peak manifests itself with increasing Au coverage. The cross section for a heavy beam contaminant scattering from Au is relatively large, and this would allow even small contaminants to be observed (see Chapter 2).

The problem should now be easy as the analyzing magnet will only bend beams that satisfy Eq. 3-2. Thus, any beam with the same $\sqrt{mE}/q$ as singly charged, 2.5 MeV He,

$$\frac{\sqrt{mE}}{q} = \sqrt{10}, \quad (A-1)$$

is a possible beam contaminant. Unfortunately for our search, this apparently eliminates the reasonable beam contaminants.

Another attempt was made with spectra acquired similar to the one shown in Fig. A-1 but for several different scattering angles. The impurity peak location was

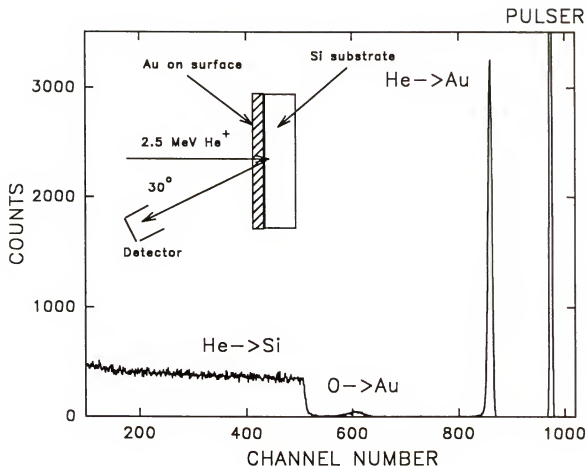


Figure A-1. Backscattering spectrum for He^+ incident on $\sim 300 \text{ \AA}$ Au on a thick Si substrate. The Au and Si signals are clearly evident with an extra peak evident between the two. This peak is due to a small O component in the incident beam, and represents about 0.4% of the incident beam.

noted at each angle. The energy of the peak at one angle divided by the energy of the peak at another angle was compared to the corresponding kinematic factor ratio for a given trial beam impurity. This removes the uncertain energy before scattering in the identification process. Such an analysis led to the conclusion that the impurity peak was oxygen, but how this beam could pass through the analyzing magnet along with the primary helium beam was still a mystery; different charge states of oxygen change the resultant beam energy, and a resulting O beam that could be bent along with helium didn't appear possible (Eq. A-1).

Our findings are corroborated by Ref. [Picr73]. They found that singly charged oxygen ions, accelerated along with the helium and having an energy the same as that of the helium beam, have a second electron stripped before reaching the analyzing magnet. This allows the beam to be bent along with the primary helium beam. Such a beam explains the impurity peak position if one considers the additional energy lost by the O (compared to He) in penetrating the dead layer of the detector. According to Ref. [Picr73], the oxygen arises from sputtering in the quartz bottle containing the helium plasma (at the top of the accelerating potential) and from ionization of molecular species present in vacuum systems.

We can estimate the size of the impurity by comparing the peak size from O and He scattering off Au and considering the difference in cross section. We find that the oxygen beam represents about 0.4% of the incident beam. The size of the impurity is of extreme importance for us because heavy ions can cause substantial irradiation damage to our Si single crystals, ruining the quality of our channeling. However, the amount of impurity observed has not noticeably affected our channeling minimum yields. As an additional precaution, we typically collect

data in sensitive crystal orientations first to minimize potential irradiation effects from the impurity beam as well as the primary helium beam.

APPENDIX B PREPARATION OF SILICON THIN WINDOWS

Essential to the research in our laboratory is the preparation of silicon thin ($\sim 8000 \text{ \AA}$), self-supporting windows to allow transmission of an ion beam. In this appendix, the procedure for making the thin windows is outlined, and the subsequent cleaning procedure immediately before putting the samples under vacuum is described. The production of the thin windows follows closely the procedure due to Cheung [Cheu80a], and the cleaning procedure is found in Ref. [Ishi86]. The technique yields high crystalline quality windows with $< 10\%$ thickness variation over the approximately 6 mm diameter window. The success rate of the procedure is about 80%.

Boron Diffusion

The silicon thin windows are created by a dopant-selective etch. Thus, there are basically three steps involved in the process. The silicon wafers (standard 2 inch diameter Si(100) or Si(110) wafers purchased from a vendor such as Virginia Semiconductor, thickness roughly $400 \mu\text{m}$) are first doped with boron spun onto the wafer (polished side) and diffused into the sample at 1100°C to a concentration of at least $\sim 5 \times 10^{19} \frac{\text{atoms}}{\text{cm}^3}$. The furnace is a 1400°C furnace (Thermo Products Corporation) and the spin-on boron is Allied Signal Accuspin spin-on dopant. The length of diffusion is, of course, related to resulting window thickness, but our control over the thickness is rather limited due to imprecision in wafer position in the furnace.

An oxide is placed on the wafers in a separate step after the diffusion. The following are the various steps in the procedure.

Assign diffusion batch number and record wafer information.

Turn water on.

Turn furnace on and record time.

The settings F:000 C:645 R:005 give a temperature of $\sim 1100^{\circ}\text{C}$ after a few hours.

Clean the wafers.

Use glass beakers for sulfuric acid and plastic beakers for hydrofluoric acid.

(A) Pre deionized water (DI) rinse

(B) $2 \text{ H}_2\text{SO}_4 : 1 \text{ H}_2\text{O}_2$ (70 ml per part) 6 min

(C) DI—leave wafers in until ready for spin on (when furnace is up to 1100°C)

(D) DI rinse for 1 min

(E) 10% HF (200 ml H_2O , 50 ml HF) 1 min

(F) DI rinse for 1 min (wafers should be hydrophobic)

Run N_2 at 3.5 liters/min through furnace to purge system.

Allow spin on boron to come to room temperature.

Purge eyedropper with DI and then boron.

Spin water off 3000 rpm for 15 sec (pump on and valve off for vacuum).

Spin boron on 3000 rpm for 20 sec (put boron on chuck to get both wafer sides).

Check spin on for spots and overall uniformity.

Load wafers onto boat so that temperature is uniform.

Sample surface should be perpendicular to gas flow, and dummies should be placed outside samples.

N₂ at 4 l/min for (slow) insertion of wafers into furnace.

Put samples in front of furnace and wait for organics to dispel.

Put samples in center of furnace to start diffusion.

N₂ at 2 l/min during diffusion.

Record length of diffusion and turn furnace off.

Clean wafers.

(A) DI for 1 min

(B) HF (same batch as used above) for 1 min

(C) DI for 1 min (wafers should be hydrophilic)

Turn furnace on and record time.

The settings F:000 C:384 R:005 give a temperature of ~ 850°C.

Keep temperature between 800 and 850°C using furnace breakers.

Load samples into boat parallel to gas flow and use dummies.

N₂ at 4 l/min for insertion of wafers into furnace.

Follow Table B-1 for gas, flow rate, and duration.

Wet O₂ is obtained by flowing gas through hot DI.

Table B-1. Gas, flow rate, and duration for oxidation step.

Gas	l/min	# min
N ₂	1.5	5
dry O ₂	2.0	5
wet O ₂	2.0	30
dry O ₂	1.5	2
N ₂	1.5	∞

Clean wafers.

(A) DI for 1 min

(B) 10% HF (new mixture) for 1 min

(C) DI for 1 min (wafers should again be hydrophobic).

Chemical Etch

The next step is to etch most of the thick silicon wafer. First, the 2 inch diameter silicon wafers are cleaved into $1\text{ cm} \times 1\text{ cm}$ square pieces (or diamond shaped pieces if the wafers are Si(110); the shape is determined by the cleaving planes which are different for the two types of wafer). Then the samples are masked in parafilm and placed on a teflon base (polished side down and on a small piece of paper) except for a circular region approximately in the center of the back of the sample (this region defines the thin window and is produced by a hole punch). A solution of 70% nitric acid, 49% hydrofluoric acid, and glacial acetic acid in the ratio of 4:2:1 etches silicon at the rate of approximately $20\text{ }\mu\text{m}$ per minute. The etch is quickly stopped when a microscope light shines through the silicon wafer, indicating a remaining thickness of several microns. The light appears purple at this point. A slow etching step that is stopped by boron concentrations exceeding $5 \times 10^{19}\text{ atoms/cm}^3$ is then performed consisting of anhydrous ethylenediamine, water, and catechol (pyrocatechin) in the ratio 10:5:(2 grams). The final window appears dark brown (thicker windows) or yellow (thinner samples).

Cleaning Procedure

The thin windows must now be cleaned just before being placed under vacuum. The cleaning procedure is outlined below and takes roughly three hours to

complete. First, organic contaminants are cleaned off, followed by metallic contaminants. Then, the idea is to place a thin (several monolayers) oxide layer on the surface that will protect the surface of the sample until it is ready to be used for experiments. Further, it is not difficult to remove this oxide under vacuum and have a clean surface by heating with a heat lamp.

- (1) Acetone cold 10 min
 - (2) Methanol hot 10 min
 - (3) Deionized water (DI 1 and 2 30 sec each)
-

- (4) HNO_3 hot 10 min
 - (5) DI
 - (6) 10% Hydrofluoric Acid dip (4 H_2O :1 HF, 50 ml per part) 30 sec
 - (7) DI
 - (8) Repeat (4) through (7) 2X (total of 3X)
-

- (9) Hot 1 NH_4OH : 4 H_2O : 1 H_2O_2 (40 ml per part) 10 min
 - (10) DI
 - (11) HF
 - (12) DI
 - (13) Repeat (9) through (12) 1X (total of 2X)
-

- (14) Hot 1 HCl : 5 H_2O : 1 H_2O_2 (40 ml per part) 10 min
- (15) DI
- (16) HF
- (17) DI
- (18) Repeat (14)

(19) DI

(20) New HF

(21) DI

(22) Hot 3 HCl : 1 H₂O : 1 H₂O₂ (50 ml per part) 10 min

(23) DI

(24) Load onto sample modules and place into introduction chamber.

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BIOGRAPHICAL SKETCH

Mark Andrew Boshart was born in Orlando, Florida, to Judith A. Auger and Ronald J. Boshart on July 15, 1969. He has two older sisters, Mary Ellen Boshart and Deborah Flanagan. Mark resided in Orlando until shortly after graduating from William R. Boone High School as Valedictorian in May 1987. He attended the University of North Carolina at Chapel Hill in August 1987. There, he pursued a bachelor's degree in Physics, graduating with highest distinction in May 1991 (17th in a class of approximately 5000). He decided to attend graduate school, and arrived at the University of Florida in August 1991, where he received a Graduate Aid in Areas of National Need (GAANN) Fellowship for his first three years. He was a Division of Sponsored Research Fellow for the following year, and a Research Assistant for his final year of graduate school. He began working for Dr. L. E. Seiberling in September 1992 studying the energy loss of channeled MeV light ions and how this can be applied to aid in studies of the Si(100) surface.

I certify that I have read this study and that in my opinion it conforms to acceptable standards of scholarly presentation and is fully adequate, in scope and quality, as a dissertation for the degree of Doctor of Philosophy.



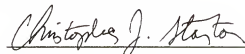
Lucy E. Seiberling, Chairperson
Associate Professor of Physics

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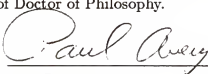
John R. Sabin
Professor of Physics

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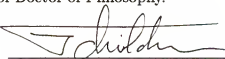
Christopher J. Stanton
Professor of Physics

I certify that I have read this study and that in my opinion it conforms to acceptable standards of scholarly presentation and is fully adequate, in scope and quality, as a dissertation for the degree of Doctor of Philosophy.



Paul R. Avery
Professor of Physics

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Jeffrey R. Childress
Assistant Professor of Materials Science
and Engineering

This dissertation was submitted to the Graduate Faculty of the Department of Physics in the College of Liberal Arts and Sciences and to the Graduate School and was accepted as partial fulfillment of the requirements for the degree of Doctor of Philosophy.

August 1996

Dean, Graduate School